JOHNS HOPKINS
APPLIED PHYSICS LABORATORY

APL PLANETARY
NUCLEAR SPECTROSCOPY

Benchmarking the accuracy of (n,n'γ) cross section libraries

Application to Planetary Nuclear Spectroscopy

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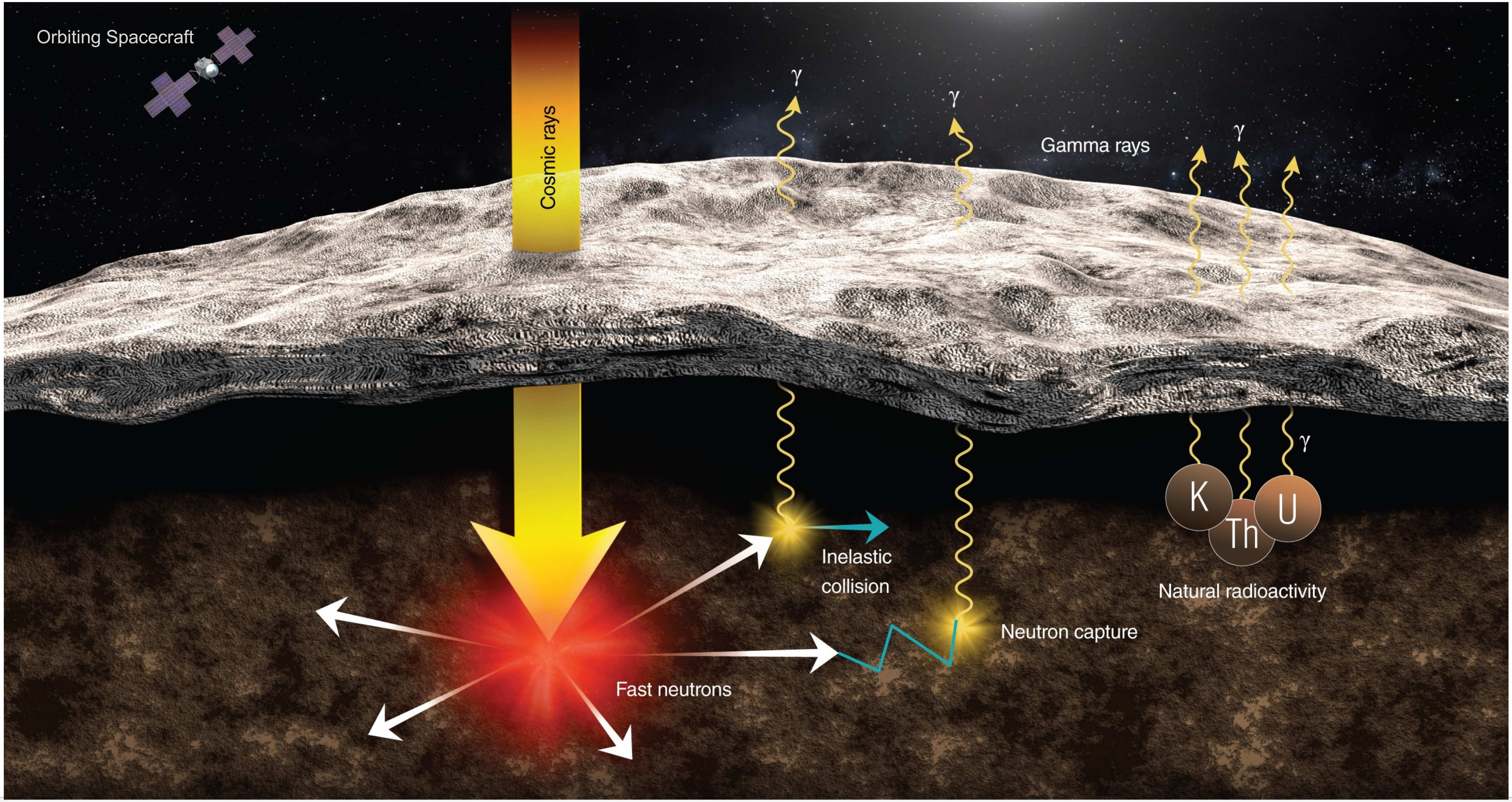
Workshop for Applied Nuclear Data Activities
2 March 2022

Introduction to planetary nuclear spectroscopy



Historical Context

- Completed/Active Investigations
  - Apollo 15 and 16 (USA)
  - Near-Earth Asteroid Rendezvous (USA)
  - Lunar Prospector (USA)
  - Mars Odyssey (USA)
  - Kaguya (Japan)
  - Chang'E (China)
  - MESSENGER (USA)
  - Lunar Reconnaissance Orbiter (USA/Russia)
  - Mars Science Laboratory (USA/Russia)
  - Mars Trace Gas Orbiter (Europe/Russia)
  - BepiColumbo (Europe/Russia/Japan)
- Upcoming Investigations:
  - LunaH Map (USA)
  - Psyche (USA)
  - MMX (Japan/USA)
  - Dragonfly (USA)
  - Commercial Lunar Payload Services (multiple payloads/missions)

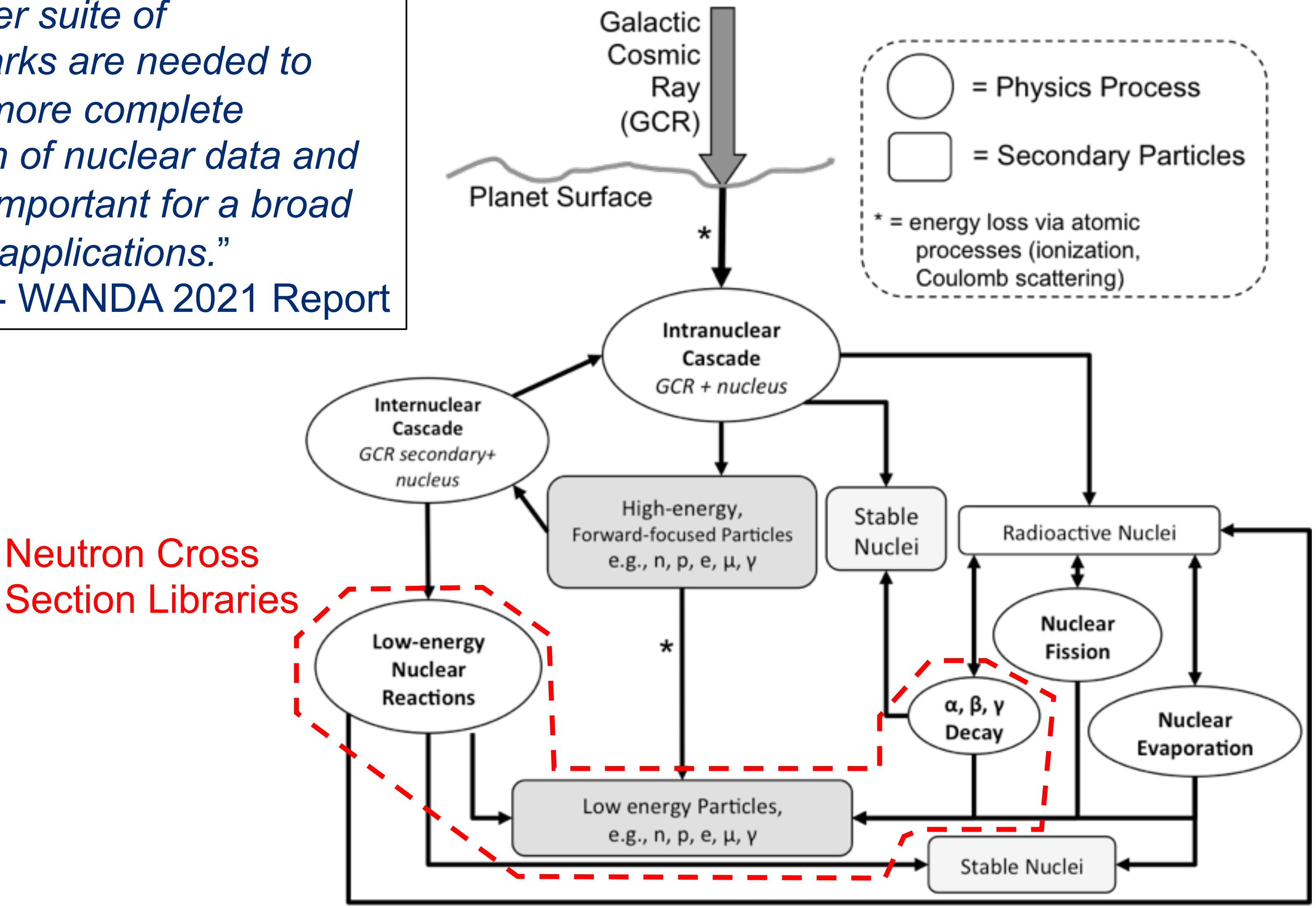
Psyche mission to metallic asteroid 16 Psyche
Launching this year (August 2022)

Nuclear spectroscopy is an active, vibrant field in planetary science.

NASA currently has numerous active and upcoming investigations valued at >$100M.

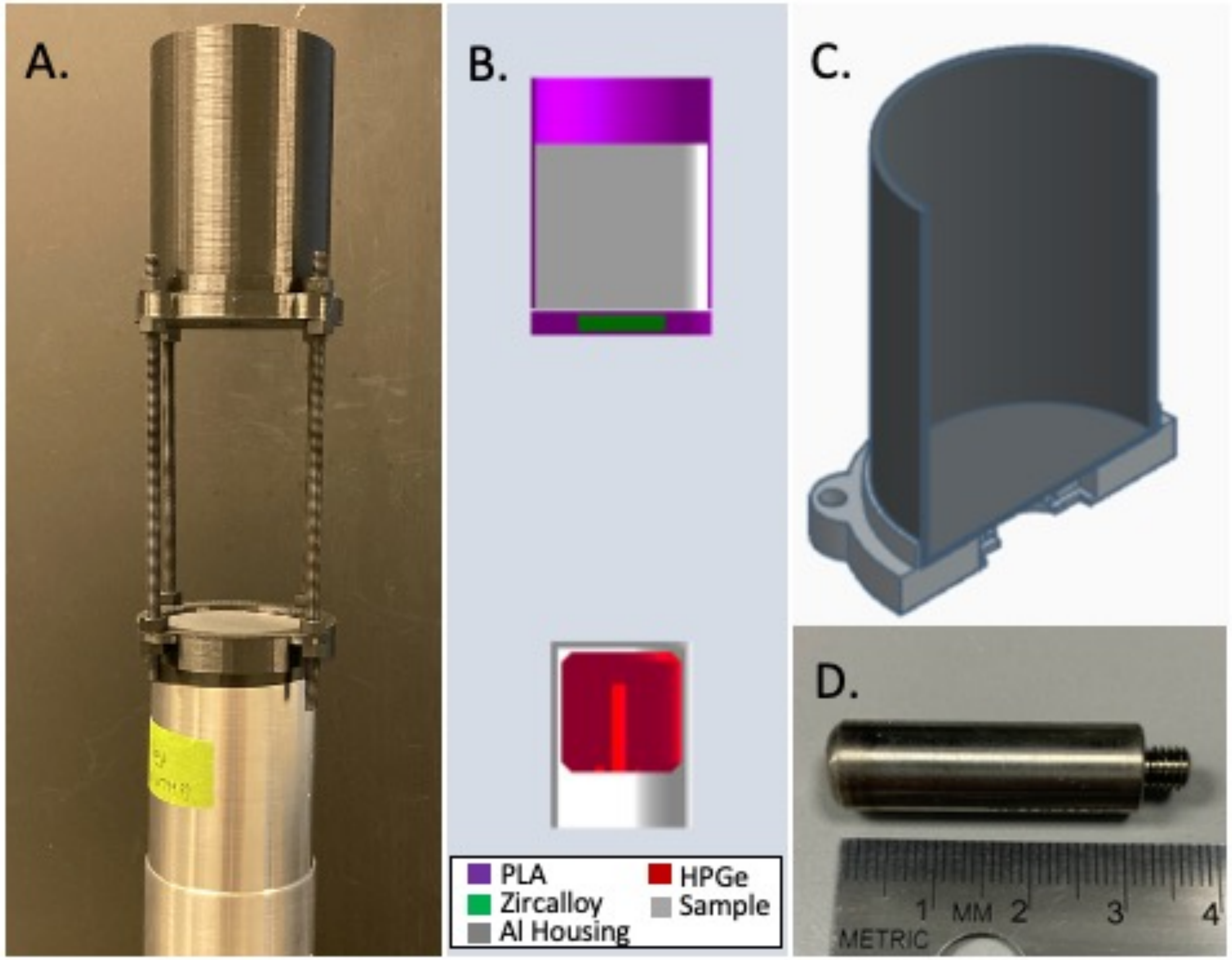
Relevant Physics Processes

> *"A broader suite of benchmarks are needed to provide more complete validation of nuclear data and physics important for a broad range of applications."*
> - WANDA 2021 Report



Benchmarking Experiment

- Measure gamma-ray emissions from neutron-irradiated samples of materials relevant for planetary neutron spectroscopy.
  - 99.9+% pure element samples
  - ^{252}Cf source, 3×10^5 n/s
  - Long (multi-day) measurements to maximize statistics
- Simple, easy-to-model measurement geometry
  - Low-mass sample cup, ~20-cm above gamma-ray sensor
  - HPGe detector w/ same size as four NASA flight instruments
- Frequent measurements of backgrounds
  - Neutron interactions w/ HPGe sensor, housing, measured weekly.

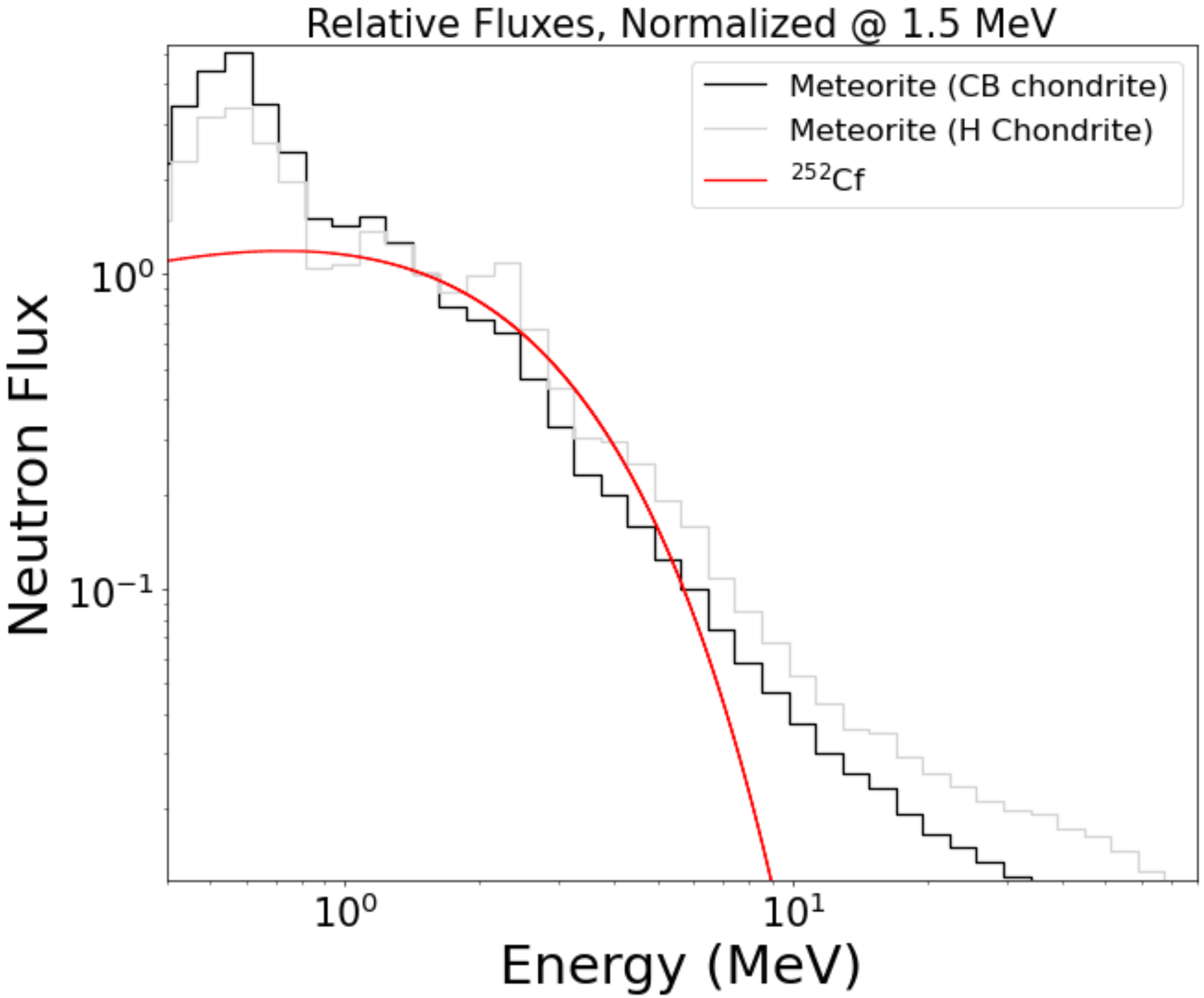


"Benchmarks are models of well-characterized experiments for which experimental uncertainties and the biases and uncertainties of any geometry and material simplifications have been assessed."

- WANDA 2021 Report

Neutron Source

- ^{252}Cf provides a similar neutron flux to that at the near-surface as produced by cosmic rays.
- Uncertainties in the ^{252}Cf neutron emission spectrum are expected to be well below the uncertainties of the gamma-ray measurements.
- A byproduct of using ^{252}Cf is copious gamma rays from fission daughters.
  - Background measurements and spectral subtraction are required to remove these gamma rays.

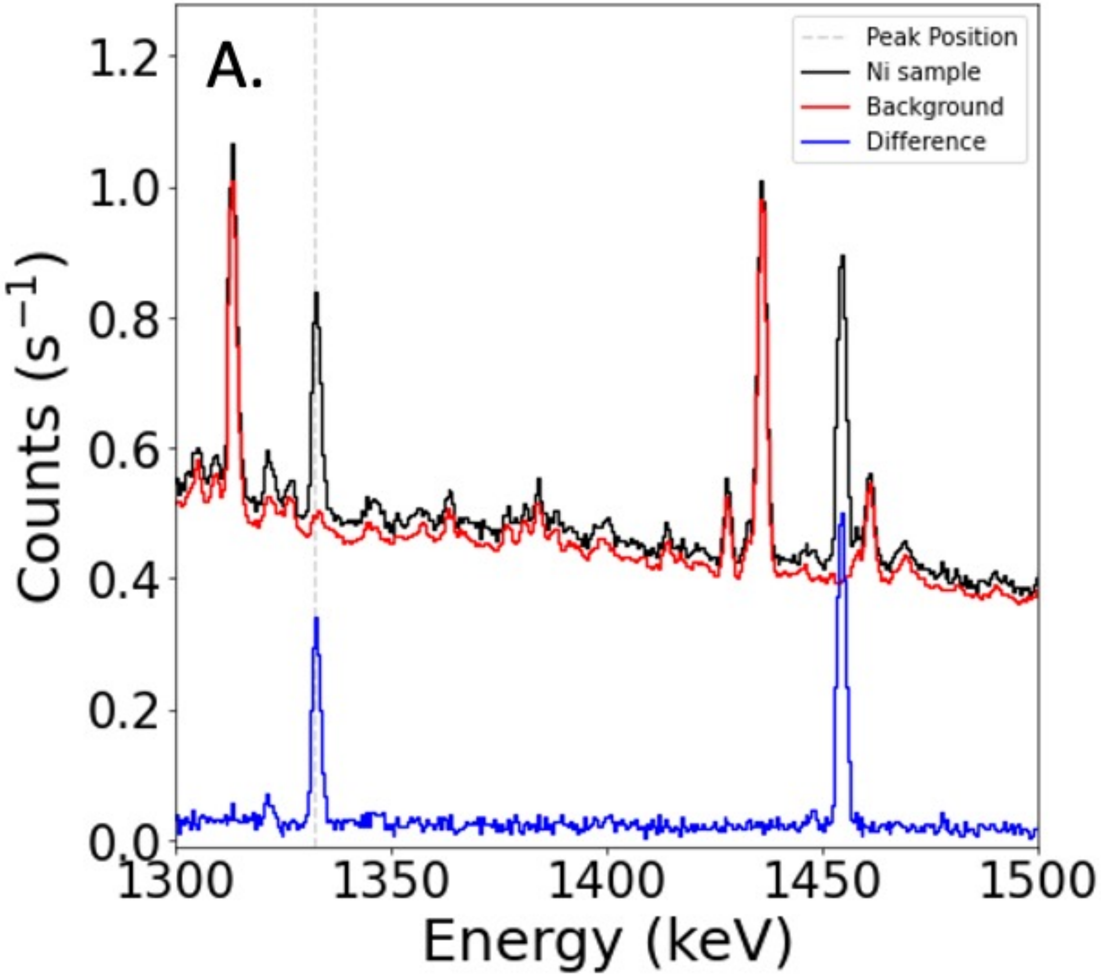


"More benchmark experiments should be performed that are similar to the Baghdad Atlas in purpose, but that have improved technology and characterization and that have fluxes similar to the application flux."

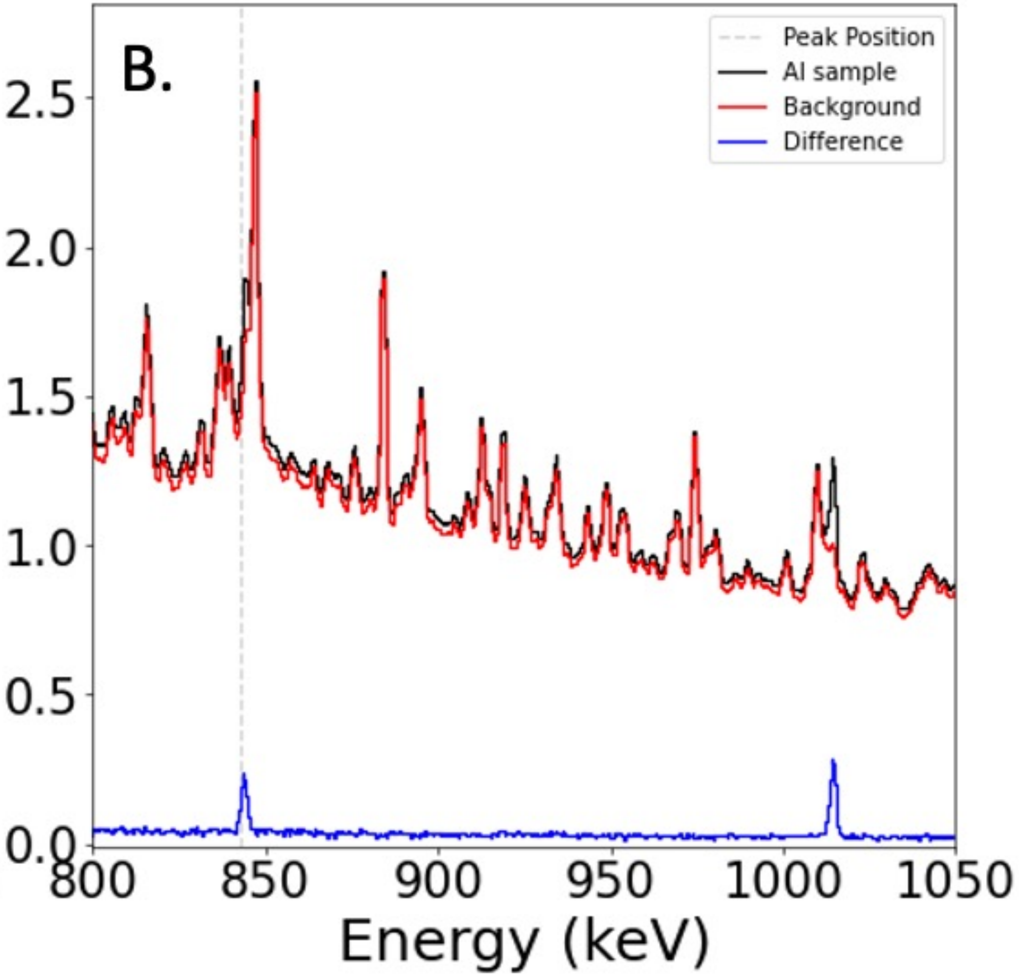
- WANDA 2021 Report

Sample Gamma-Ray Spectral Analysis

Nickel Sample Analysis



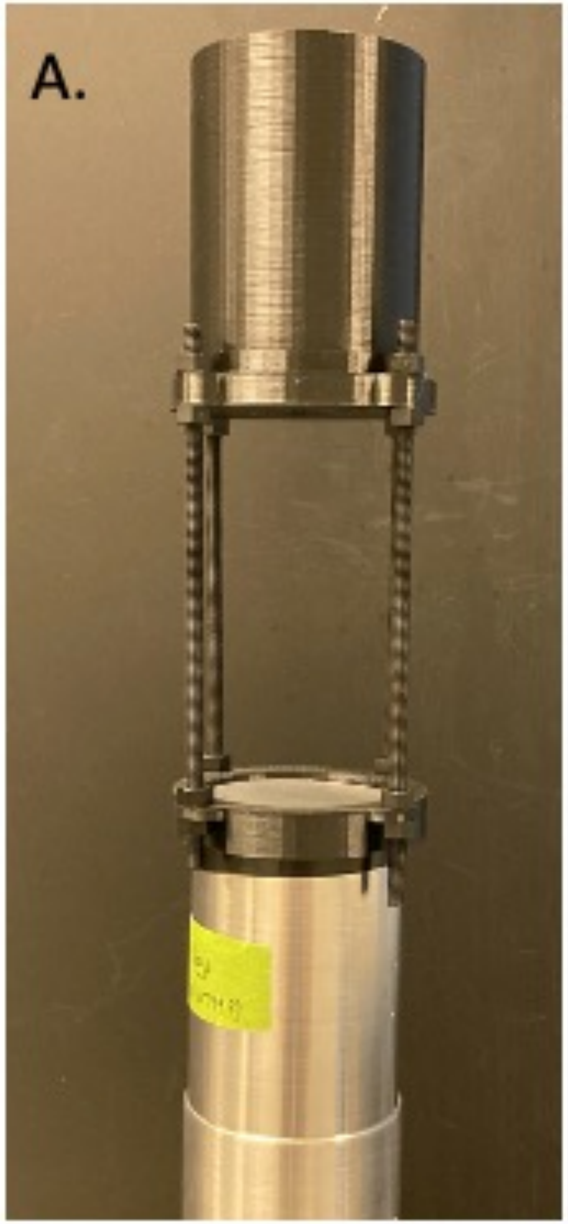
Aluminum Sample Analysis



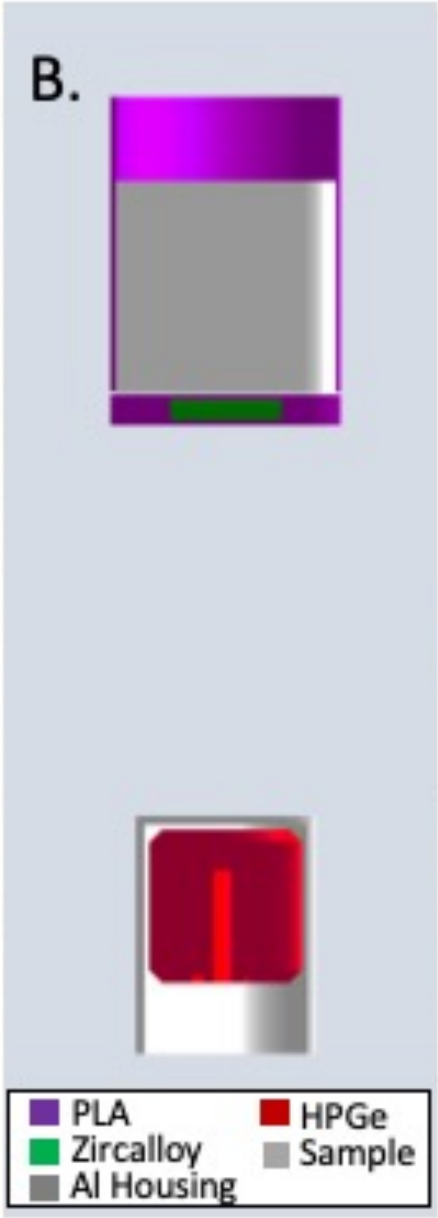
"Difference" measurements (sample – background) provide clean spectra with gamma-ray peaks that are exclusively from the (n,n'γ) reactions of interest.

Geant4 Simulations

- Geant4 simulations (see right panel of figure) include the detector, its housing, 3-D printed plastic parts, the sample, and the Cf source housing.
- For each simulation, all physics selections are identical except the neutron cross section library.
  - We used the following libraries for this study:
    - Geant4 Neutron Data Library:
      - G4NDL 4.6, G4NDL 4.5
    - Evaluated Nuclear Data Files:
      - ENDF VIII.0, ENDF VII.1, & ENDF VI
    - Japanese Evaluated Nuclear Data Library:
      - JENDL 4.0 & 3.3
    - Chinese Evaluated Nuclear Data Library
      - CENDL 3.1
    - Russian neutron data library:
      - BROND 3.1 & 2.2

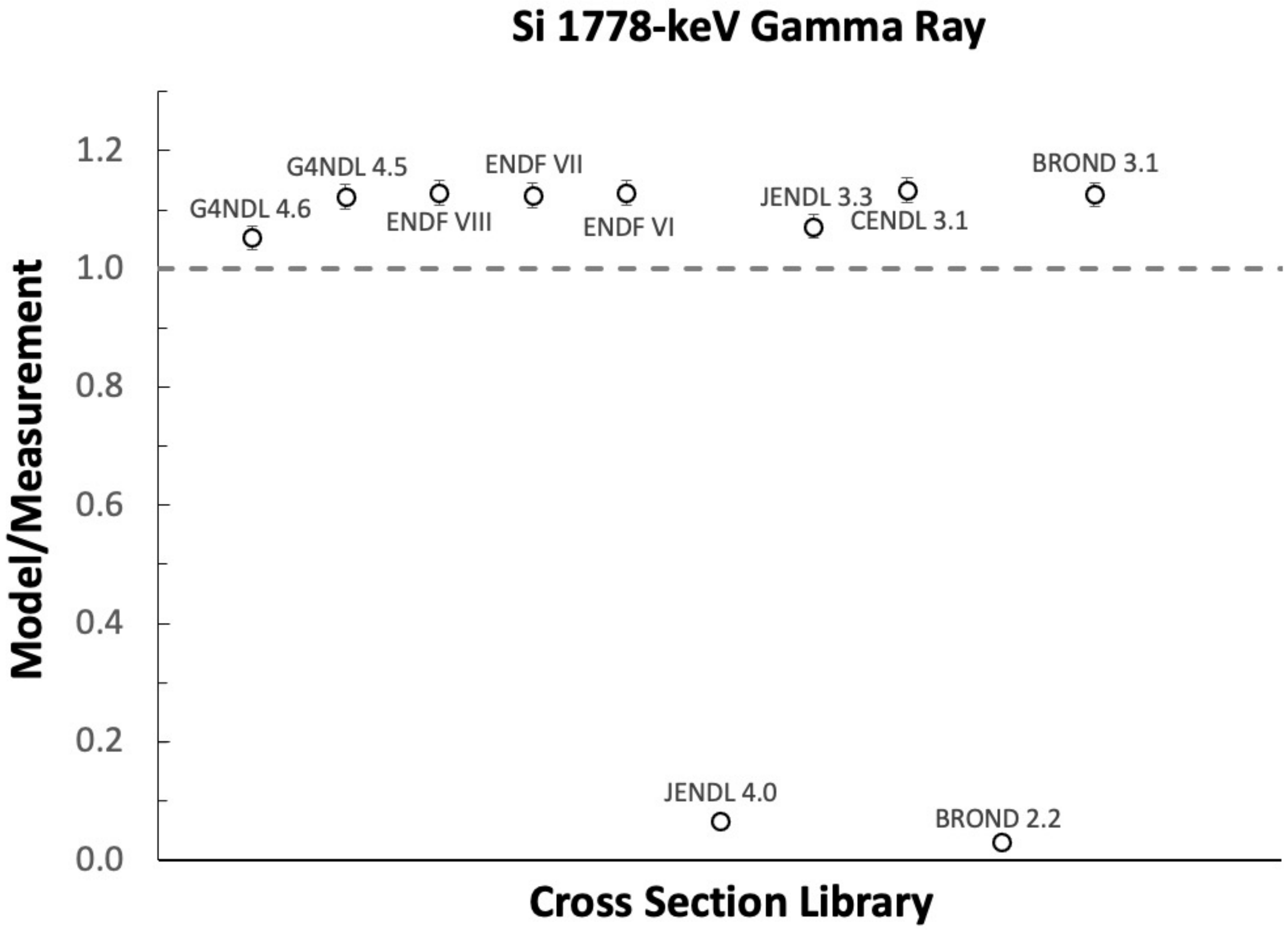


Experiment

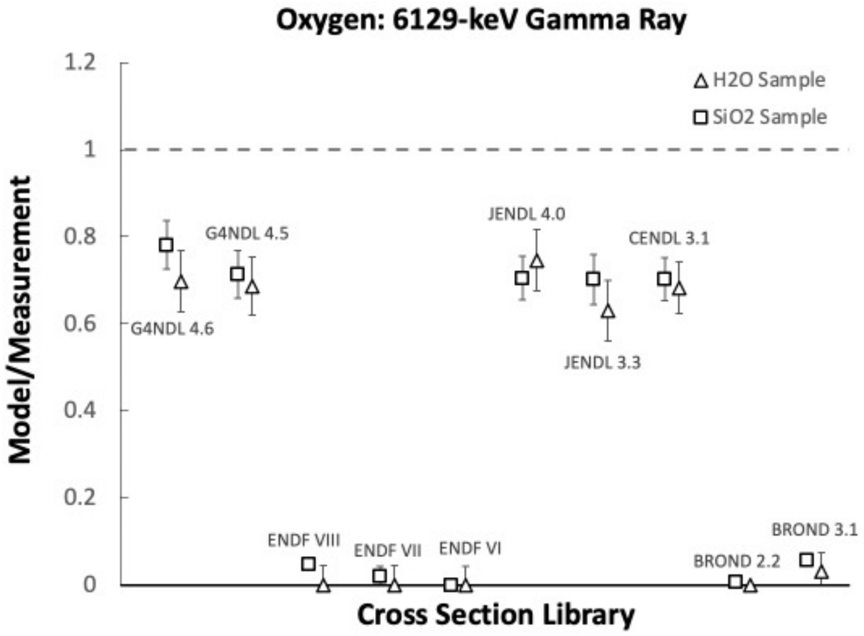


Geant4 Simulation Geometry

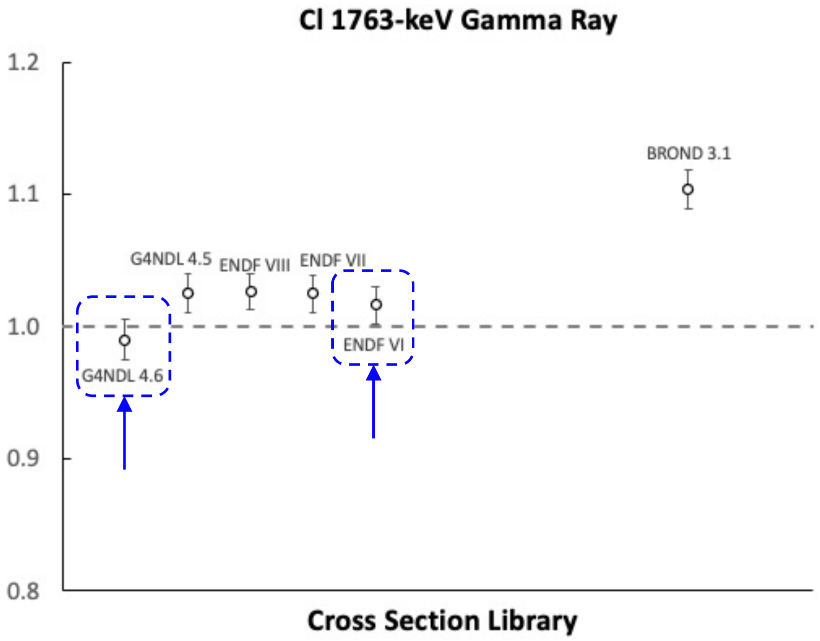
Model-to-measurement comparison



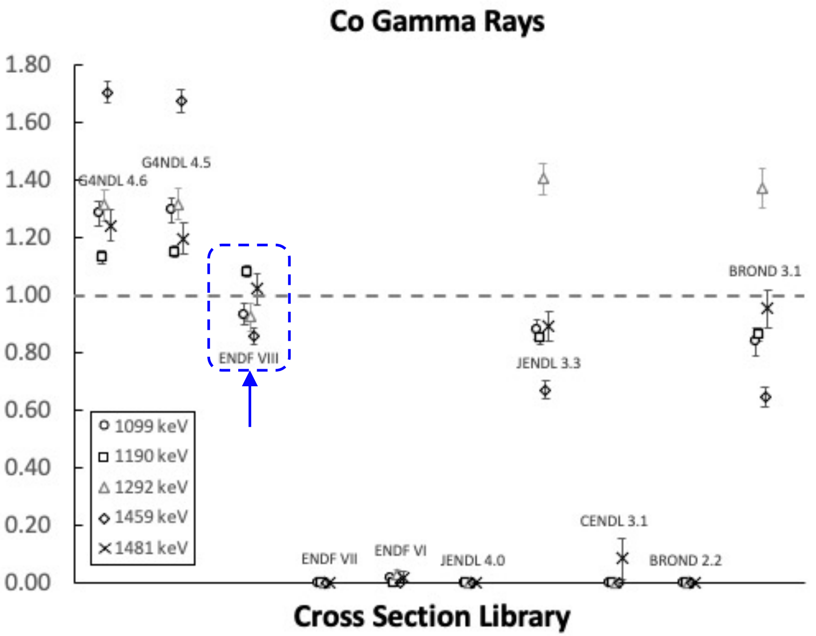
Subset of the model-to-measurement comparison



No acceptable cross section library (agreement for two separate measurements)



Two acceptable cross section libraries (G4NDL 4.6, ENDF VI)



One acceptable cross section library (ENDF VIII), agreement for multiple gamma-ray emission peaks

Summary Results

Model/Measurement Ratio

	Gamma Ray (keV)	G4NDL 4.6	G4NDL 4.5	ENDF VIII	ENDF VII	ENDF VI	JENDL 4.0	JENDL 3.3	CENDL 3.1	BROND 3.1
H	2223	1.45±0.01	1.47±0.01	1.44±0.01	1.47±0.01	1.45±0.01	1.44±0.01	1.46±0.01	1.46±0.01	1.45±0.01
O	6129	0.78±0.06	0.71±0.05	0.05±0.01	--	--	0.71±0.05	0.70±0.05	0.70±0.70	0.06±0.01
Na	440	1.13±0.03	0.45±0.01	0.25±0.01	0.25±0.01	0.25±0.01	1.26±0.03	1.26±0.03	--	1.17±0.03
	1634	1.92±0.03	1.73±0.17	--	--	--	1.66±0.02	1.69±0.02	--	2.06±0.03
Mg	1369	1.42±0.02	1.42±0.02	1.38±0.07	1.39±0.07	0.00±0.00	1.44±0.07	1.42±0.06	0.86±0.02	1.44±0.07
Al	843	1.22±0.01	1.07±0.01	1.09±0.01	1.10±0.01	1.11±0.01	1.09±0.06	1.05±0.01	1.05±0.01	1.11±0.01
	1014	1.47±0.01	1.32±0.01	1.31±0.01	1.31±0.01	1.30±0.01	1.22±0.08	1.22±0.00	1.20±0.00	1.31±0.01
	2211	1.21±0.01	1.18±0.01	1.18±0.01	1.12±0.01	1.12±0.01	1.01±0.01	0.98±0.01	0.94±0.01	1.14±0.01
Si	1779	1.05±0.02	1.12±0.02	1.13±0.02	1.13±0.02	1.13±0.02	0.07±0.00	1.07±0.02	1.13±0.02	1.13±0.02
S	2232	1.31±0.01	0.78±0.01	--	0.78±0.01	0.80±0.01	0.79±0.01	0.79±0.01	--	0.80±0.01
Cl	1763	0.99±0.01	1.02±0.01	1.03±0.01	1.02±0.01	1.02±0.01	--	--	--	1.10±0.02
Ca	3736	1.00±0.04	--	--	--	0.06±0.01	--	1.12±0.04	0.04±0.01	--
Ti	983	1.07±0.03	1.06±0.03	1.06±0.03	1.09±0.06	--	1.12±0.06	1.10±0.06	1.07±0.06	1.06±0.06
Fe	846	1.04±0.01	1.11±0.01	1.16±0.01	1.11±0.01	1.11±0.01	1.12±0.01	1.12±0.01	1.06±0.01	1.24±0.03
	1238	0.80±0.04	0.91±0.04	0.94±0.04	0.92±0.04	0.88±0.04	0.97±0.04	0.99±0.04	0.76±0.04	0.85±0.10
	1408	1.39±0.10	1.11±0.09	1.08±0.09	1.02±0.09	0.95±0.08	1.14±0.09	1.12±0.07	1.07±0.09	1.55±0.24
Co	1099	1.28±0.04	1.30±0.04	0.93±0.04	--	--	--	0.88±0.04	--	0.84±0.05
	1190	1.13±0.02	1.15±0.02	1.08±0.02	--	--	--	0.85±0.02	--	0.86±0.02
	1292	1.31±0.06	1.32±0.05	1.93±0.05	--	--	--	1.40±0.06	--	1.37±0.07
	1459	1.71±0.04	1.67±0.04	0.86±0.03	--	--	--	0.67±0.03	--	0.65±0.03
	1481	1.24±0.06	1.20±0.05	1.02±0.05	--	--	--	0.89±0.05	--	0.95±0.07
Ni	1332	1.04±0.04	1.23±0.05	1.04±0.04	1.21±0.05	1.13±0.04	0.97±0.04	0.97±0.04	1.05±0.04	1.02±0.04
	1454	0.87±0.06	0.87±0.06	1.01±0.06	0.86±0.06	0.85±0.05	0.71±0.05	0.72±0.05	0.99±0.06	0.84±0.06

(n,γ) reaction

Model Accuracy
Within 5%
Within 5-10%
Within 10-20%
Diff. >20%
"--" = No Peak in Model

Summary Results

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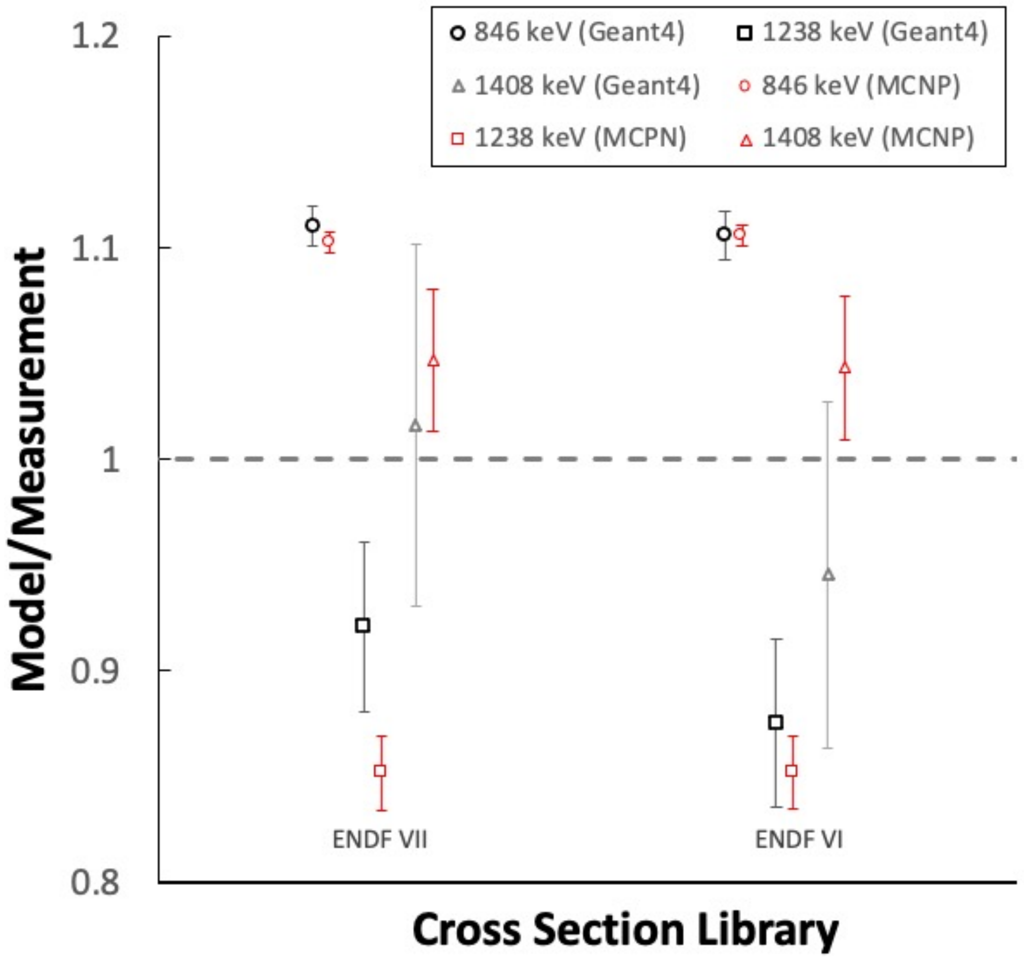
	1454	0.87±0.06	0.87±0.06	1.01±0.06	0.86±0.06	0.85±0.05	0.71±0.05	0.72±0.05	0.99±0.06	0.84±0.06

Model Accuracy
Within 5%
Within 5-10%
Within 10-20%
Diff. >20%
"--" = No Peak in Model

We can build a hybrid library to meet many of our needs. However, there are no acceptable options for ***H, O, Na, Mg, and S.***

Confirmation with MCNP

- Preliminary results suggest MCNP and Geant4 produce similar results.
  - MCNP result requires an arbitrary normalization that is not present for Geant4
  - MCNP has access to fewer neutron cross section libraries than Geant4.
- We've completed MCNP modeling for the iron sample measurements.
  - Used ENDF VII.1 and ENDF VI.8
  - Additional sample simulations in progress.
- The consistency between Geant4 and MCNP shown here suggests the measurement to model discrepancy is due to the neutron cross section libraries.



Summary

“Benchmark experiments that primarily test radiative capture (n,γ) and inelastic scattering (n,n’γ) reaction data would be the most useful for these varied applications. […] Measurements of gamma spectra would be ideal.”

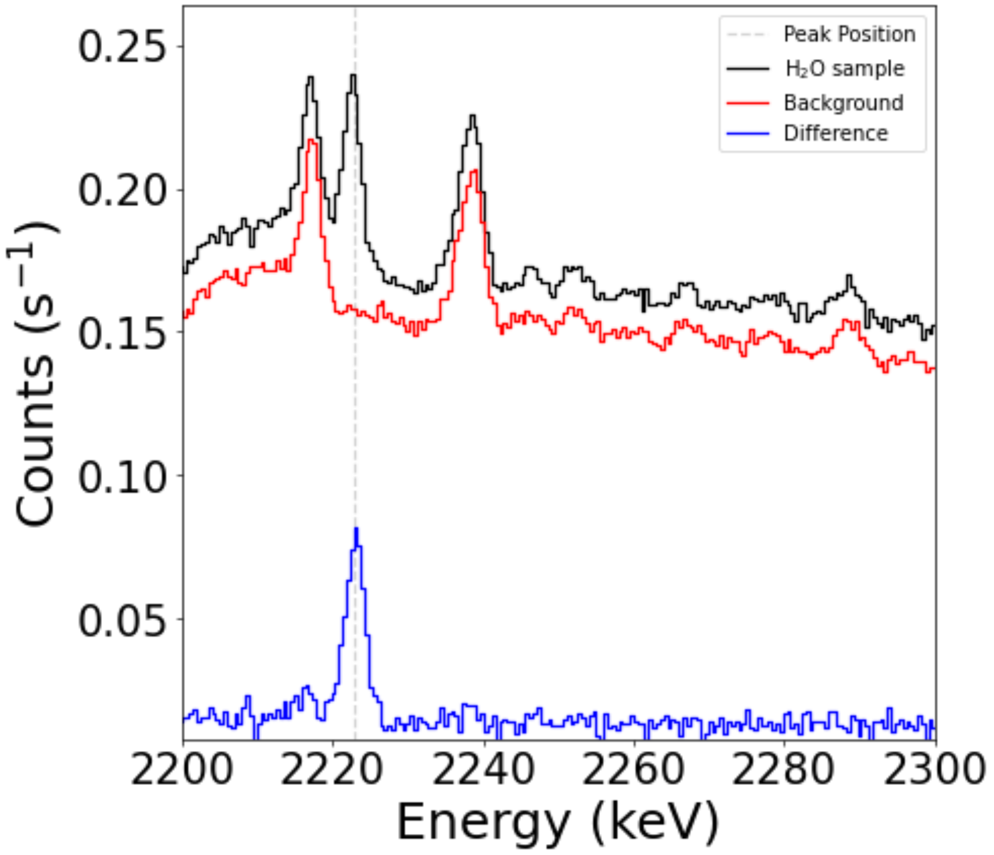
- WANDA 2021 Report

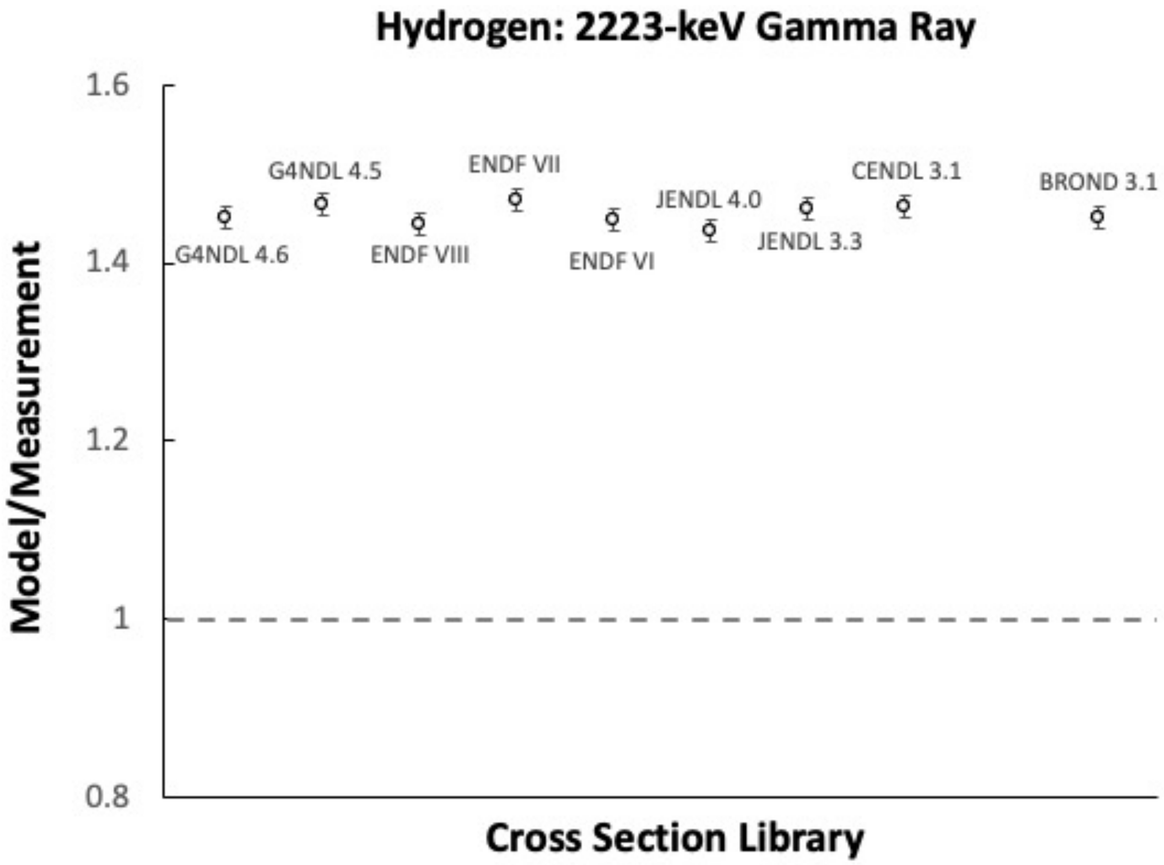
- We have conducted a series of experiments designed to provide a robust benchmark for (n,n’γ) reactions.
  - Experiments included element standards for O, Na, Mg, Al, Si, S, Cl, Ca, Ti, Fe, Co, and Ni
- The accuracy of the simulations varies strongly as a function of which neutron inelastic cross section library is used.
  - There is no single best-choice cross section library
  - For many elements (O, Na, Mg, S), there is no acceptable library choice for planetary nuclear spectroscopy experiments
- We would like to work with the neutron library developers to improve future versions of the library for our application.
  - Accurate cross sections for gamma-ray production from (n,n’γ) reactions is not always the priority for neutron library efforts.

Backup slides

- Measurements, and simulation-to-measurement comparisons for each element of interested are included in the following slides.

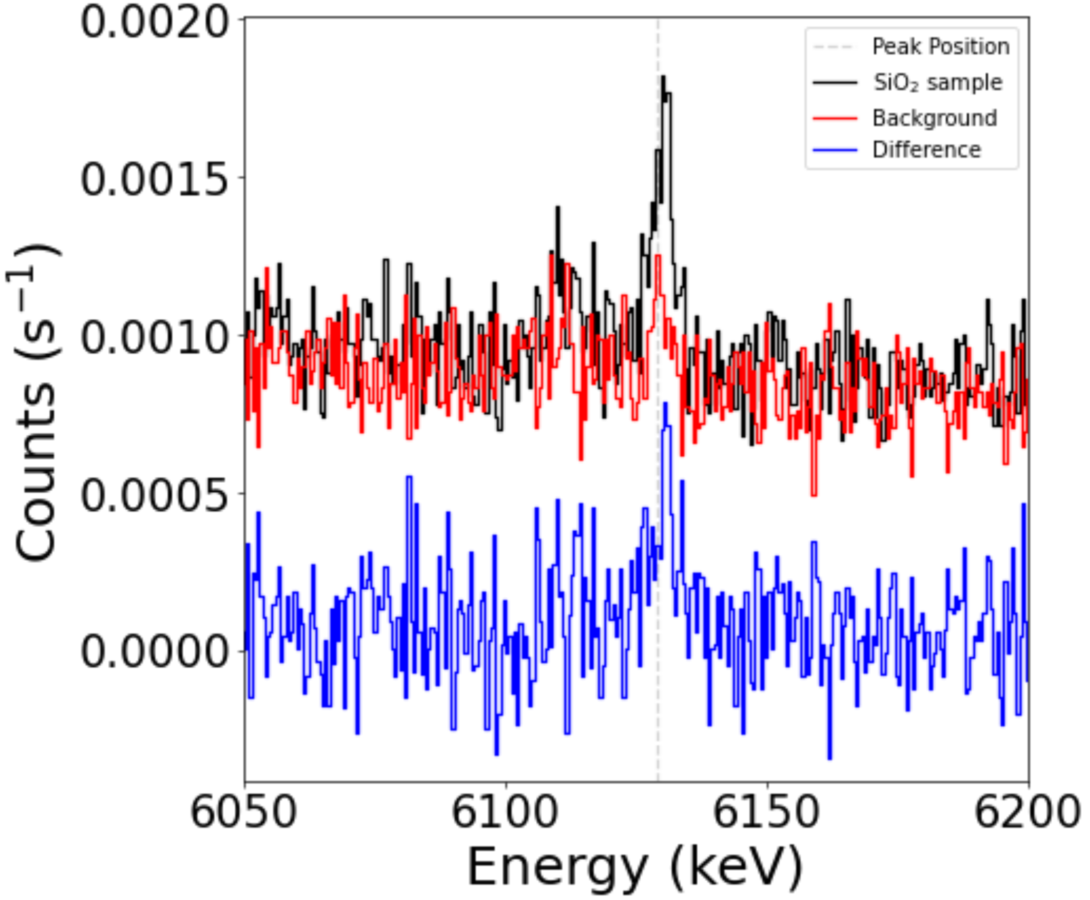
Hydrogen – 2223-keV gamma ray

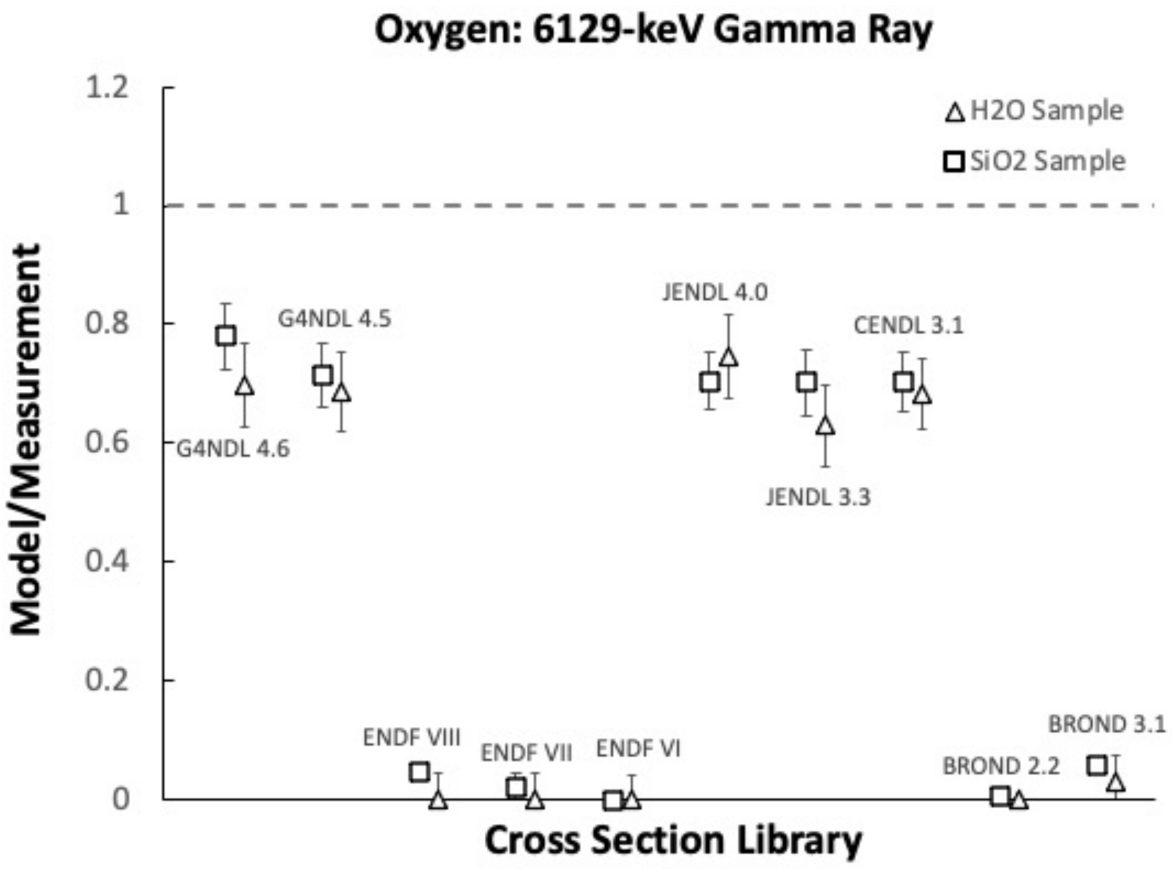




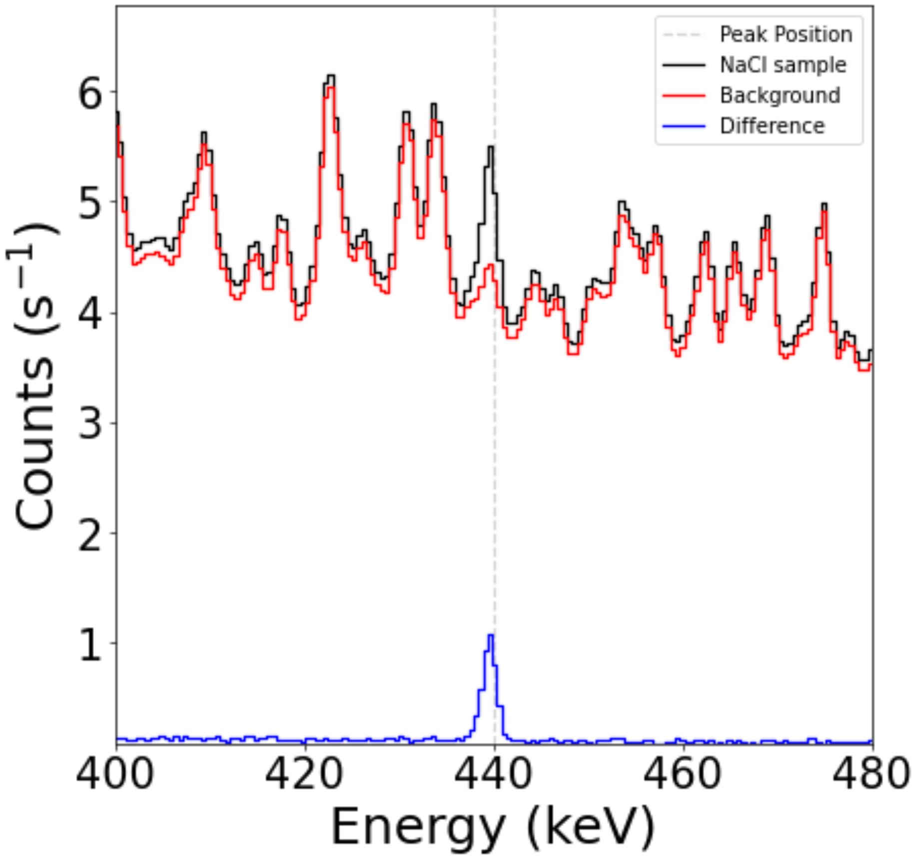
Note that, unlike all other peaks in this study, this is from neutron radiative capture reaction H(n,γ)D

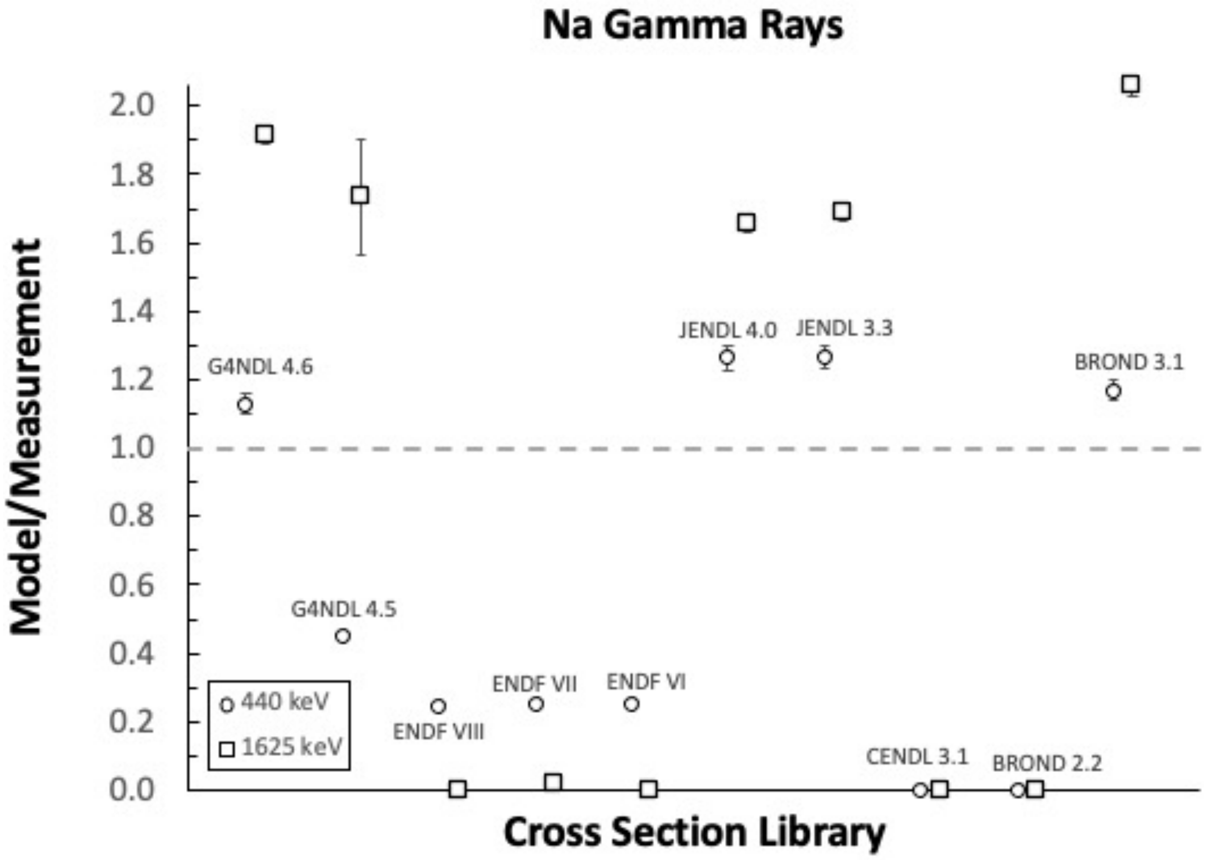
Oxygen – 6129-keV gamma ray



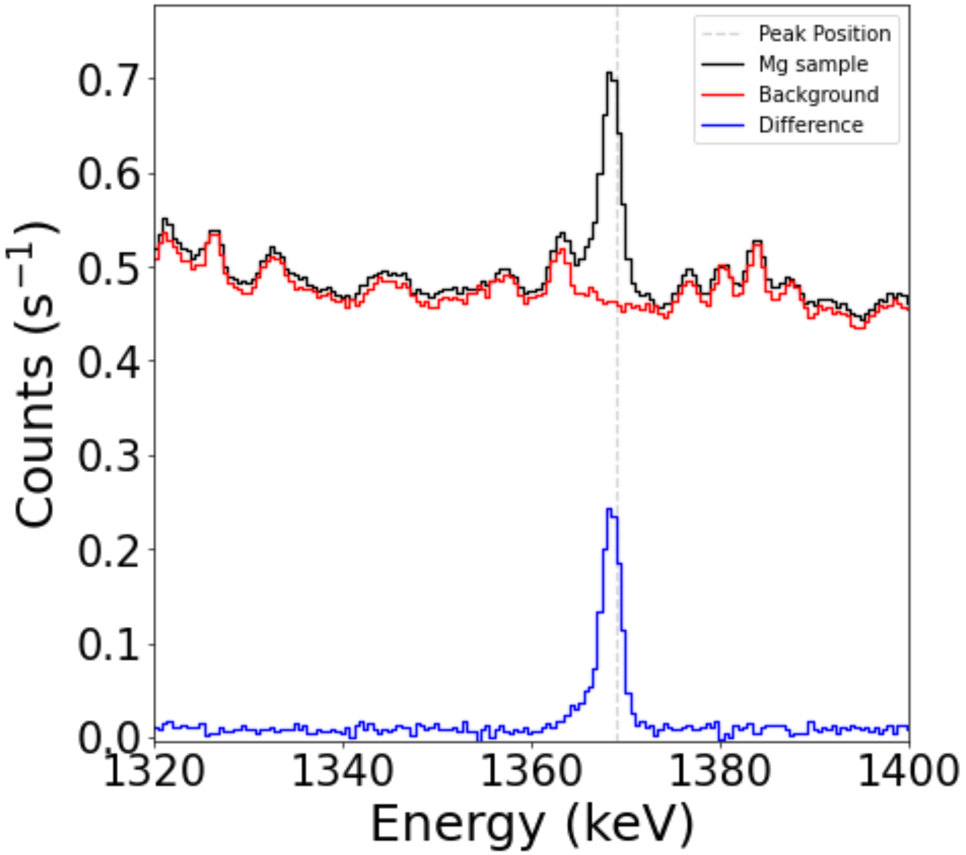


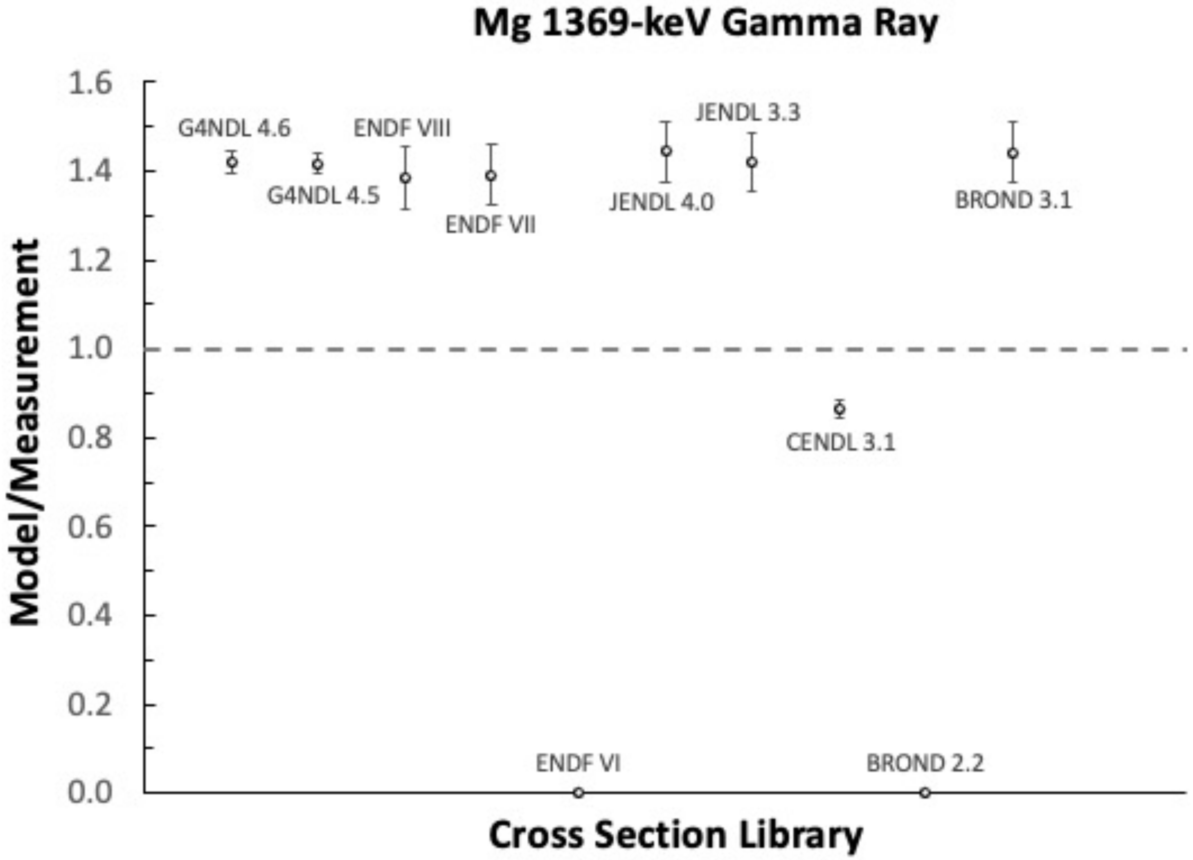
Sodium – multiple gamma rays



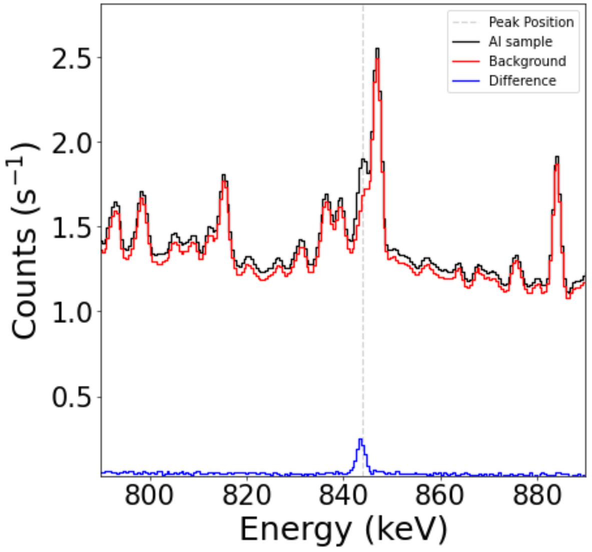


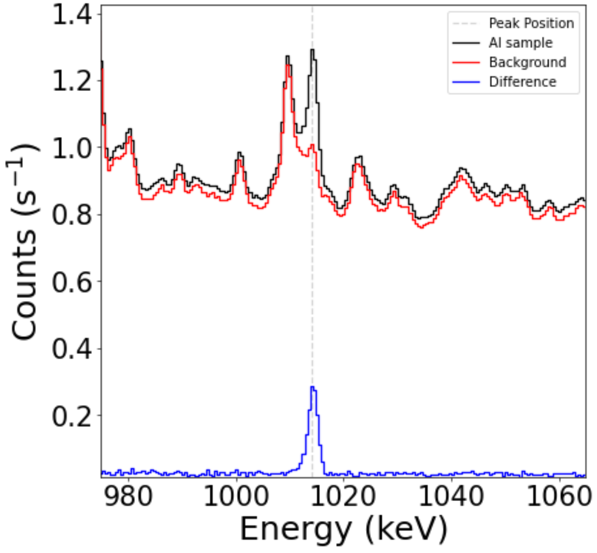
Magnesium – 1369-keV gamma ray

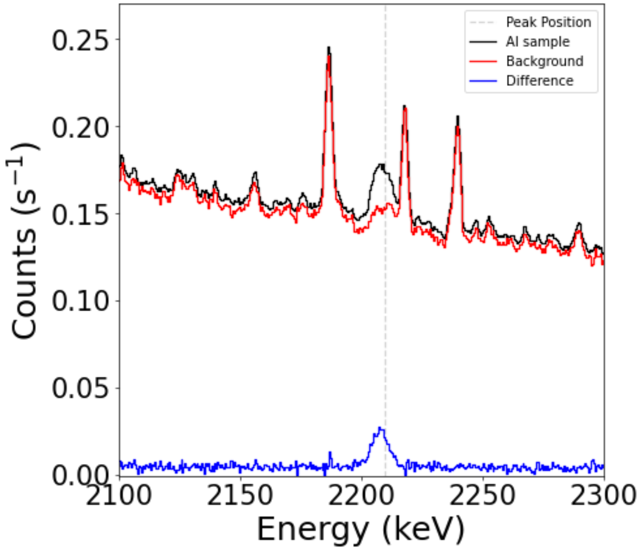


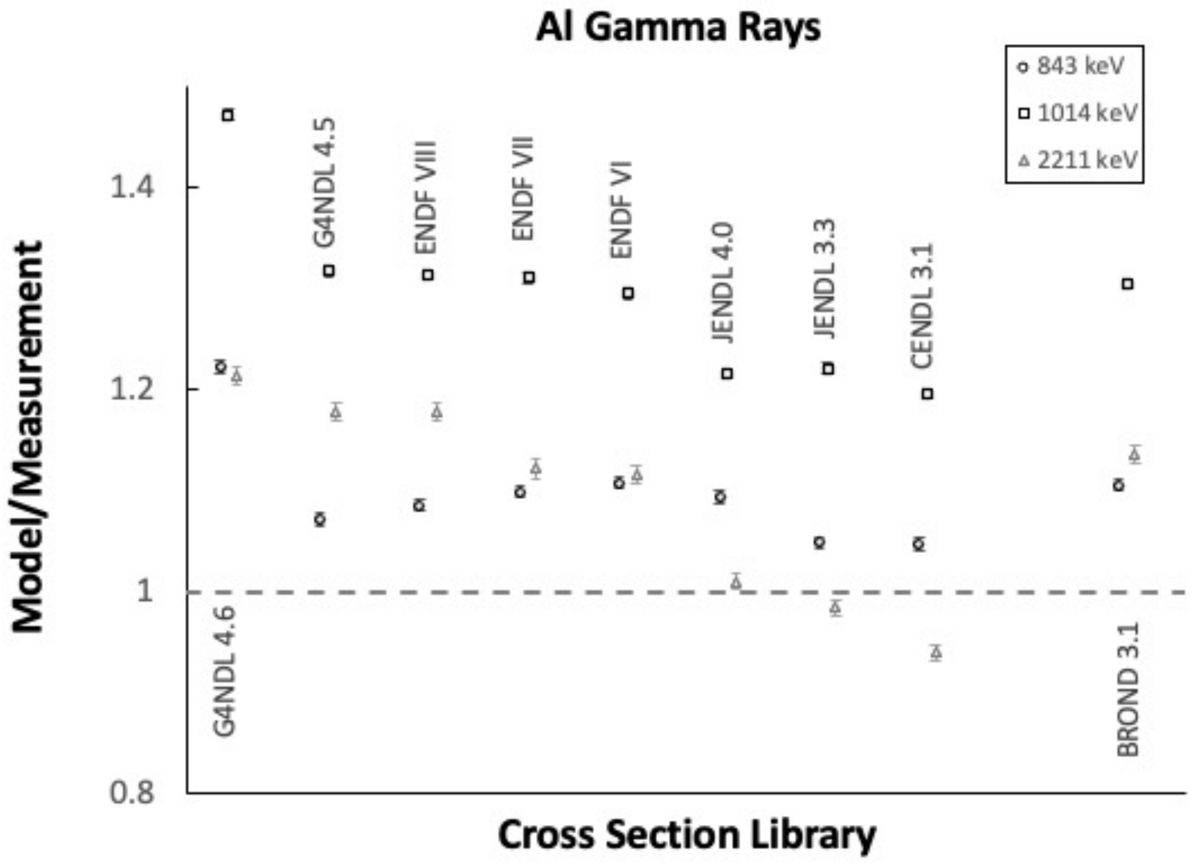


Aluminum – multiple gamma-ray peaks

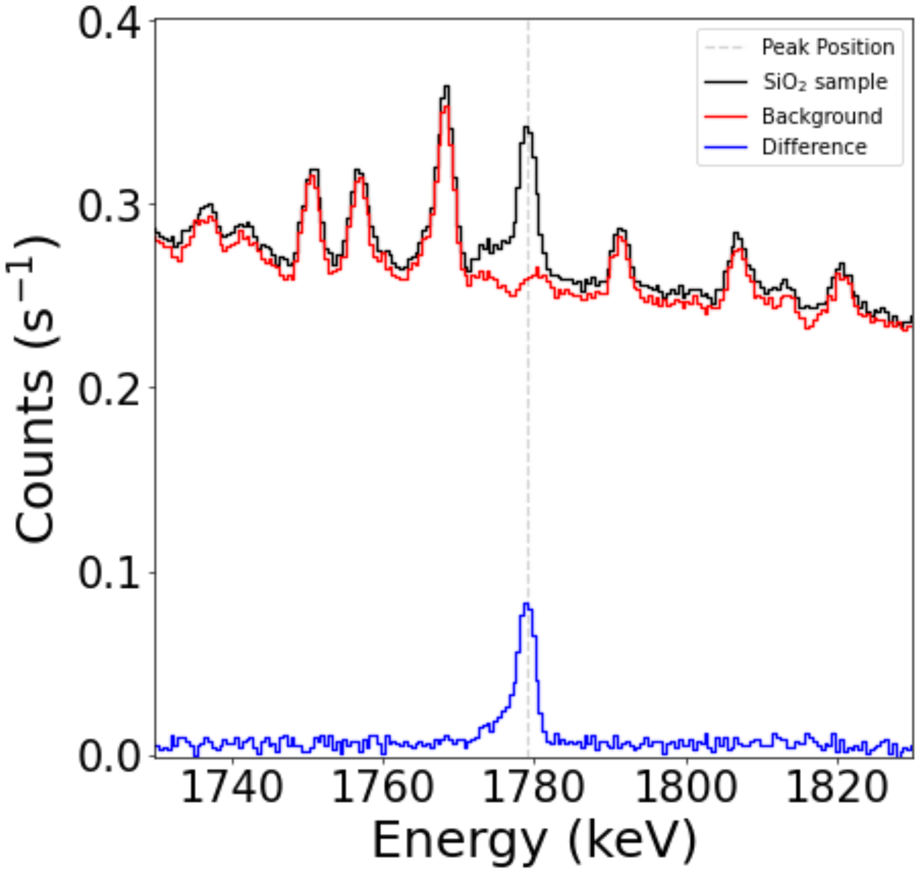


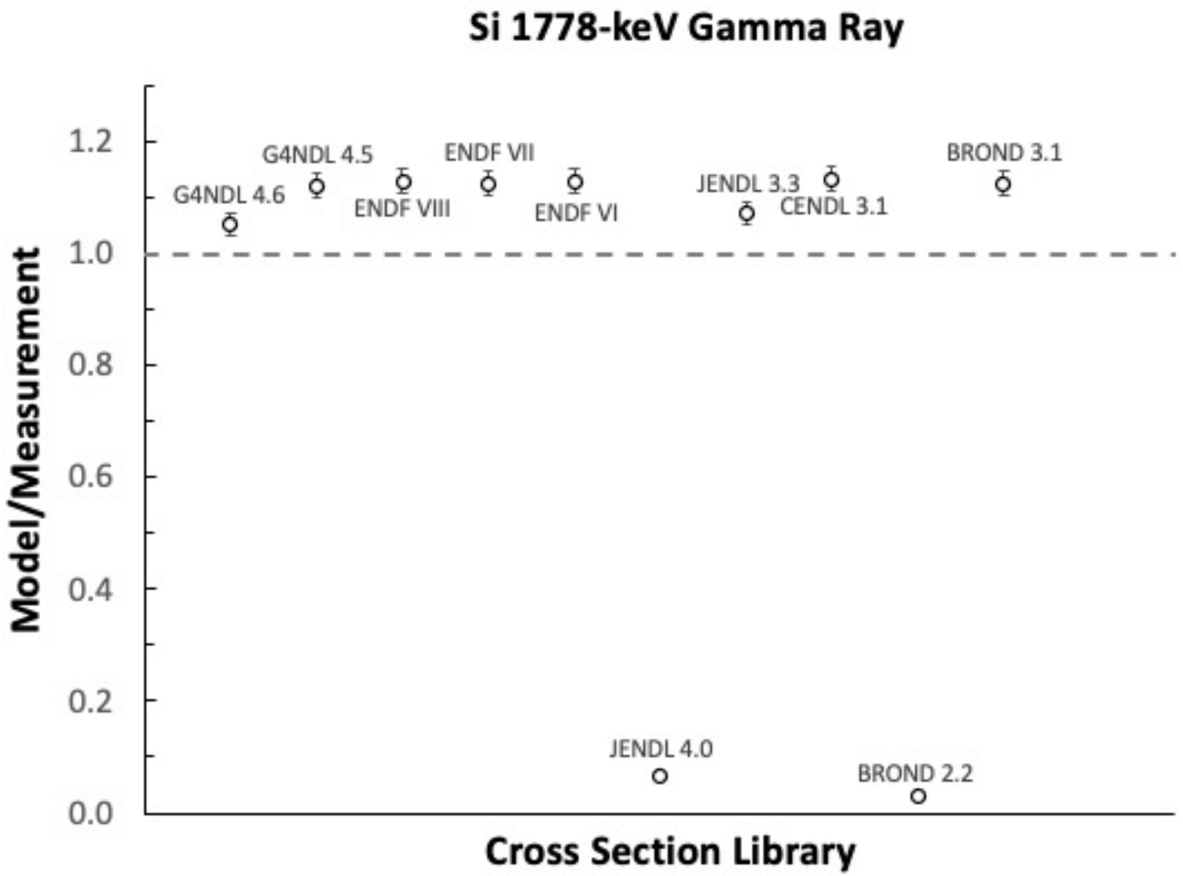




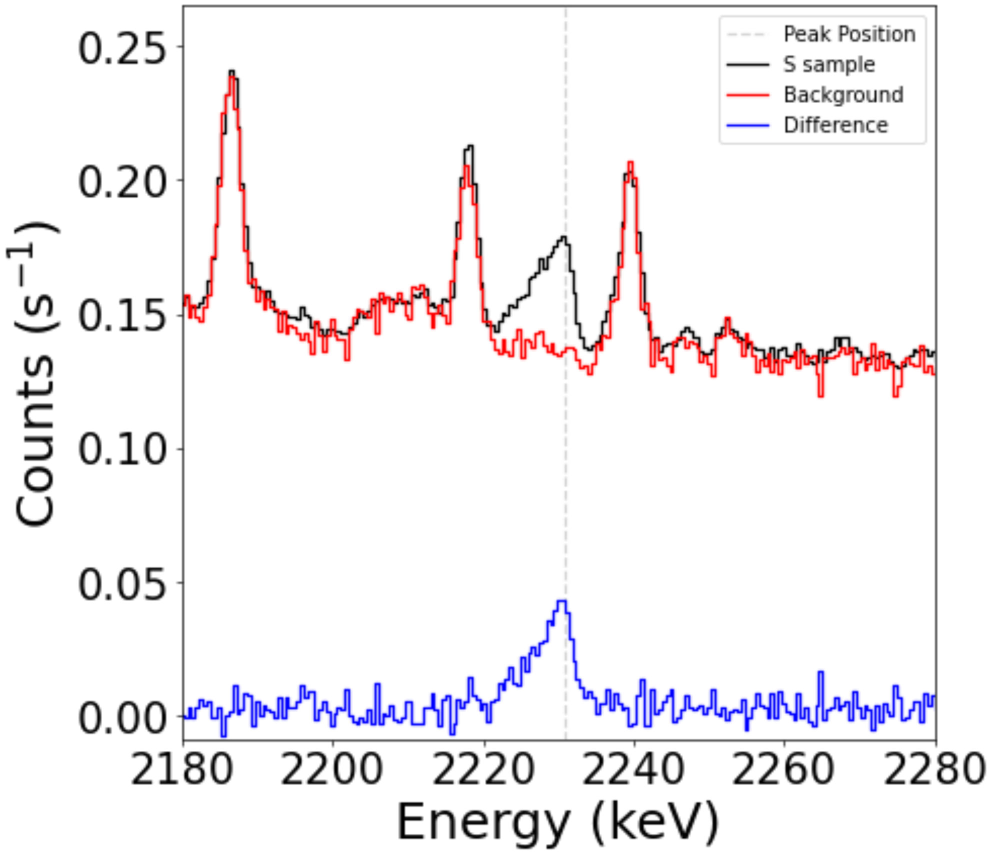


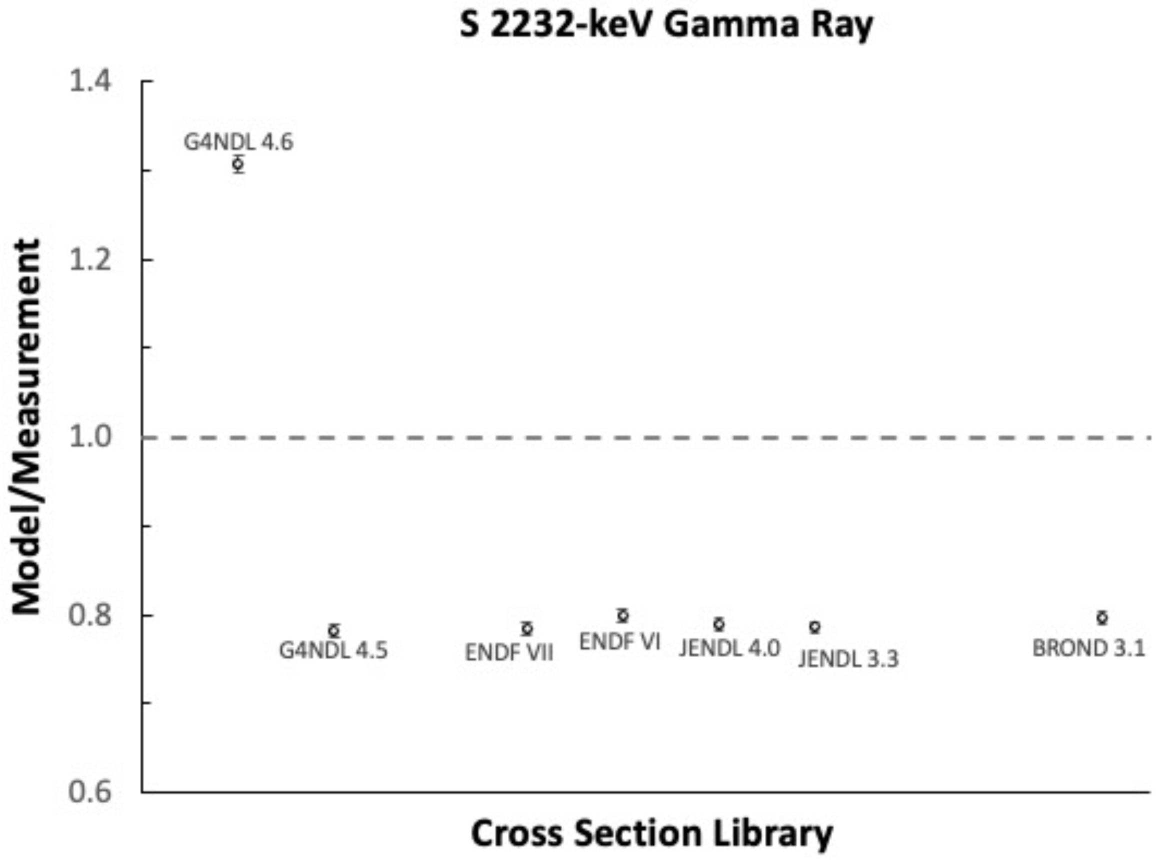
Silicon – 1779-keV gamma ray peak



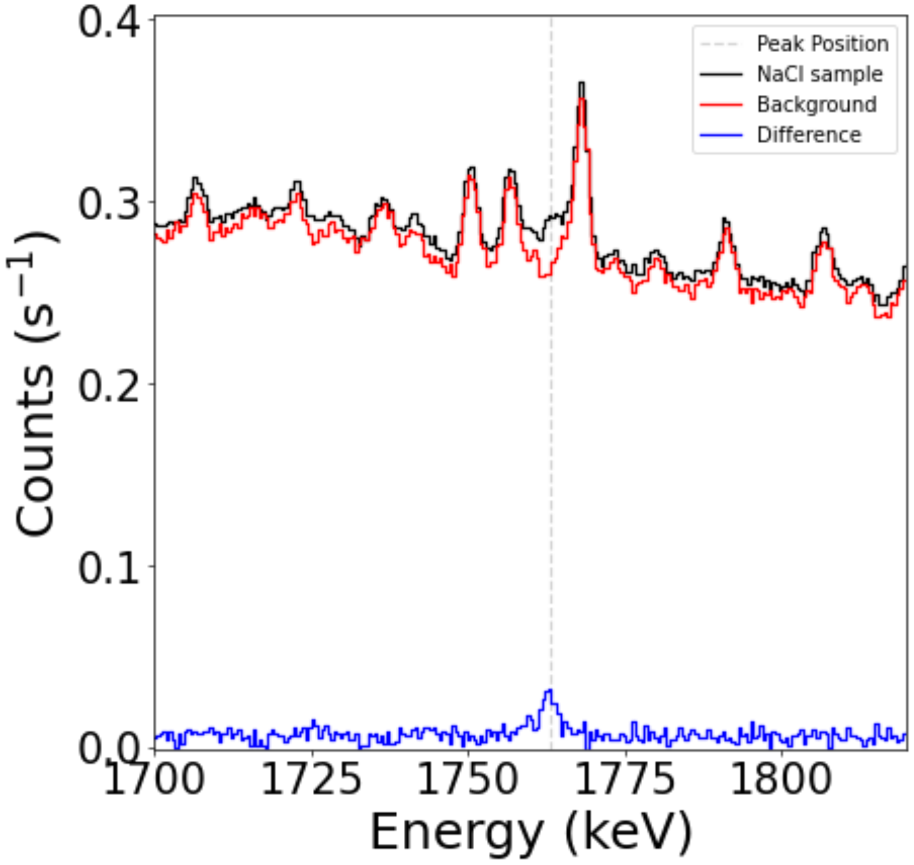


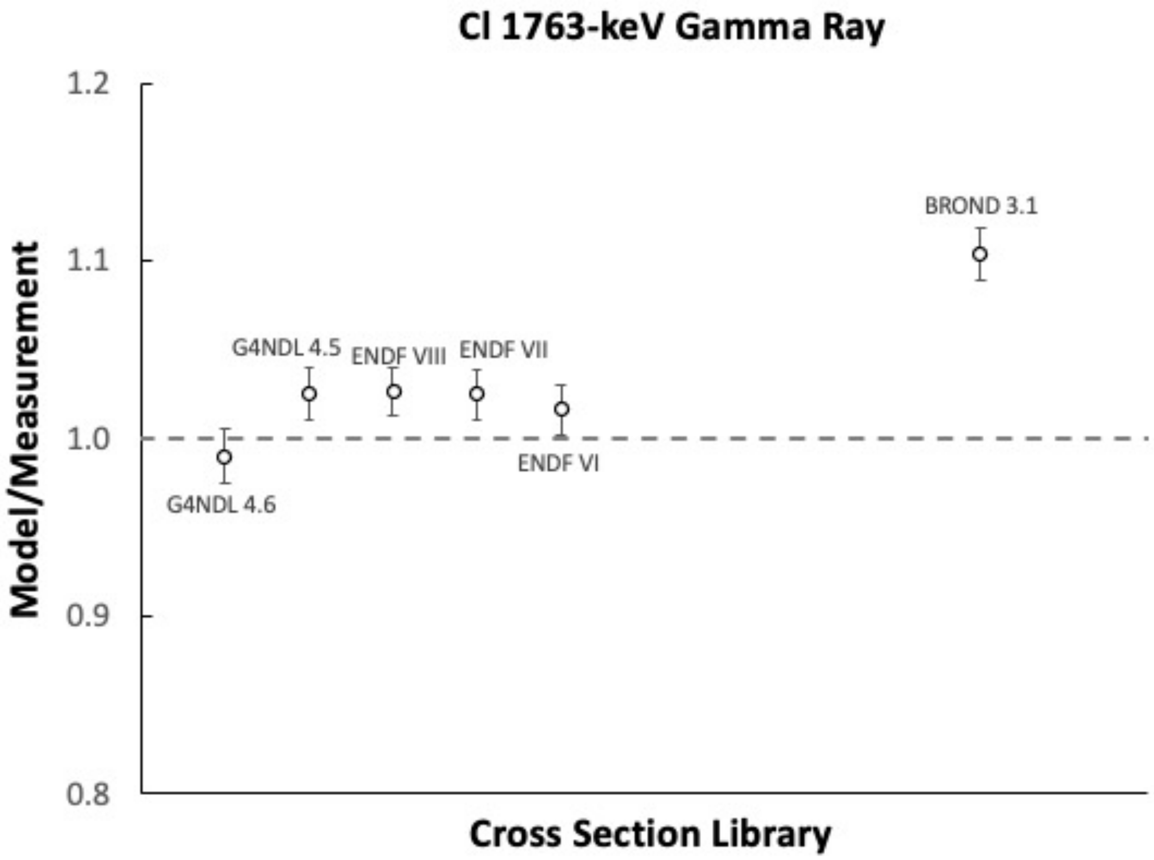
Sulfur – 2231-keV gamma ray



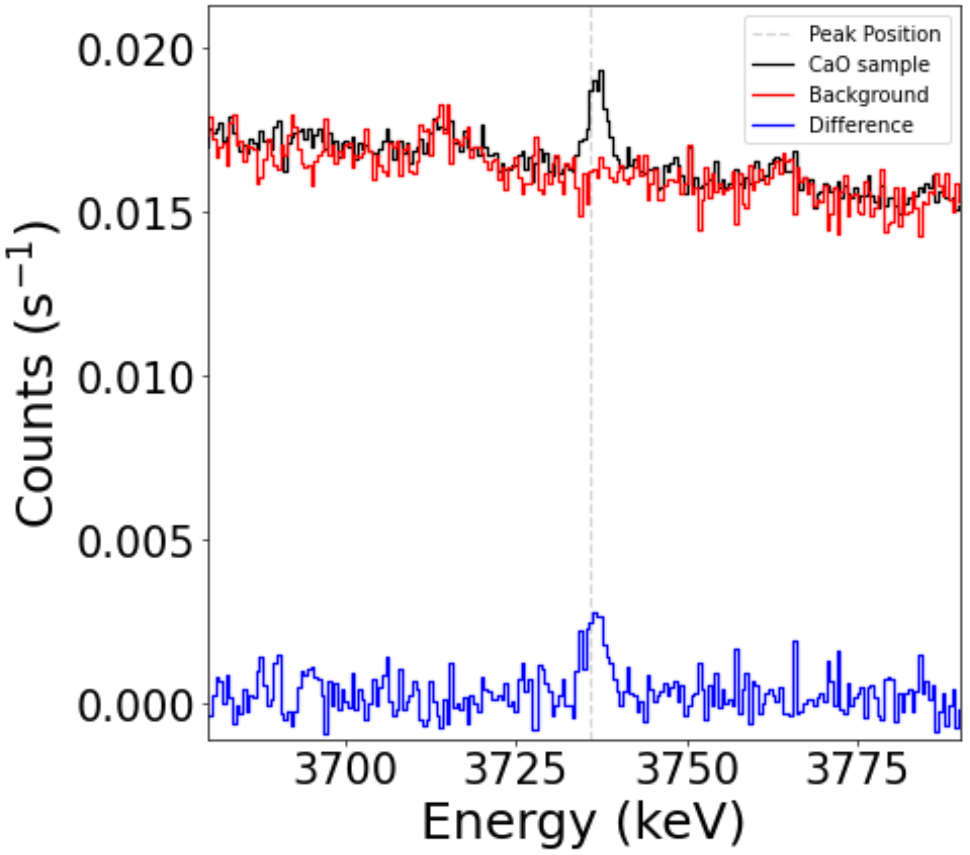


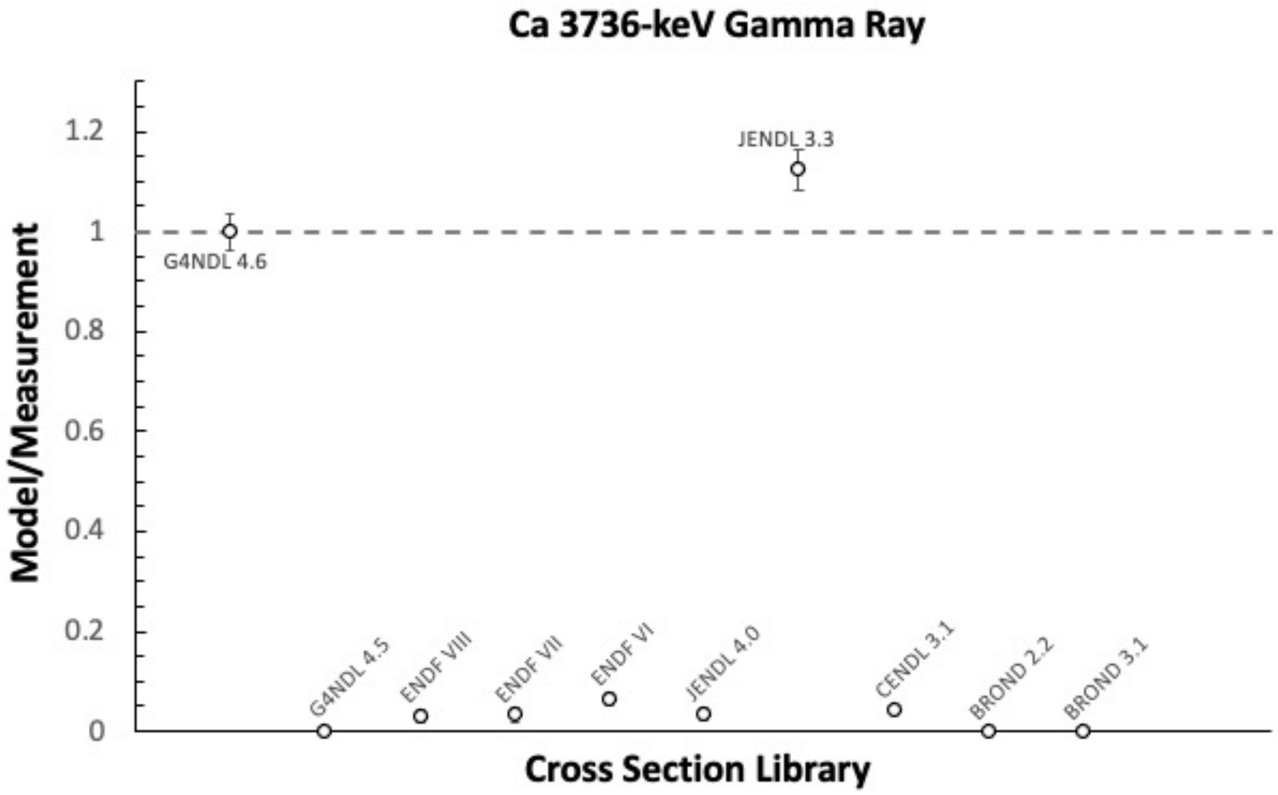
Chlorine – 1763-keV gamma ray



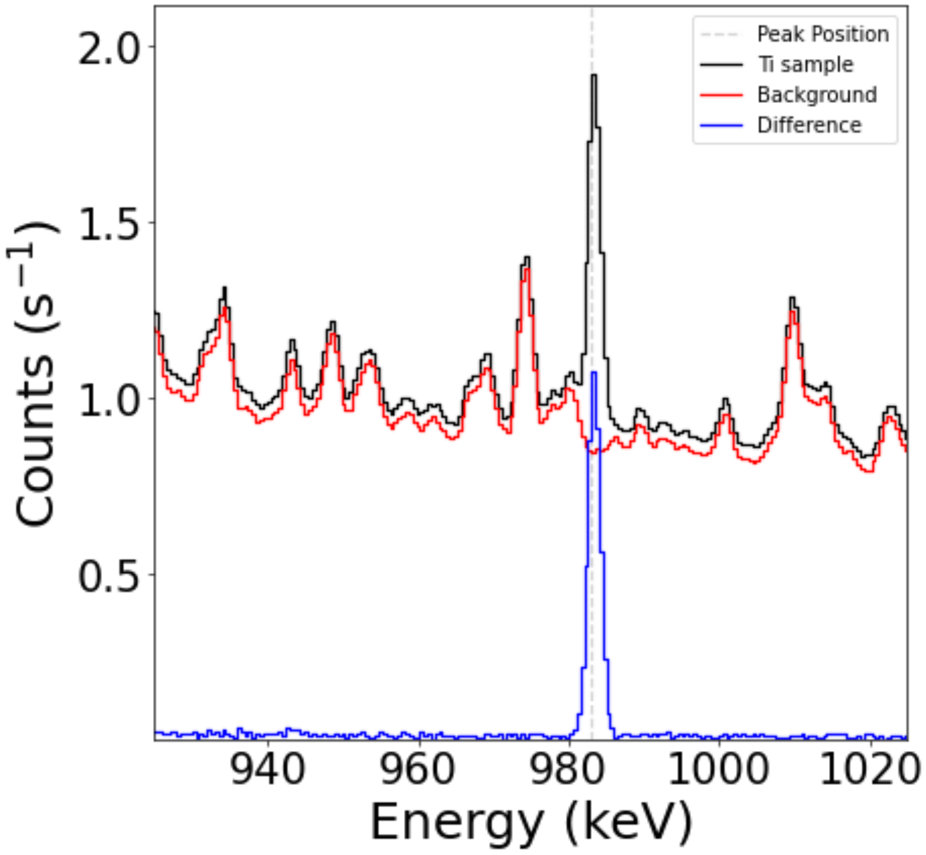


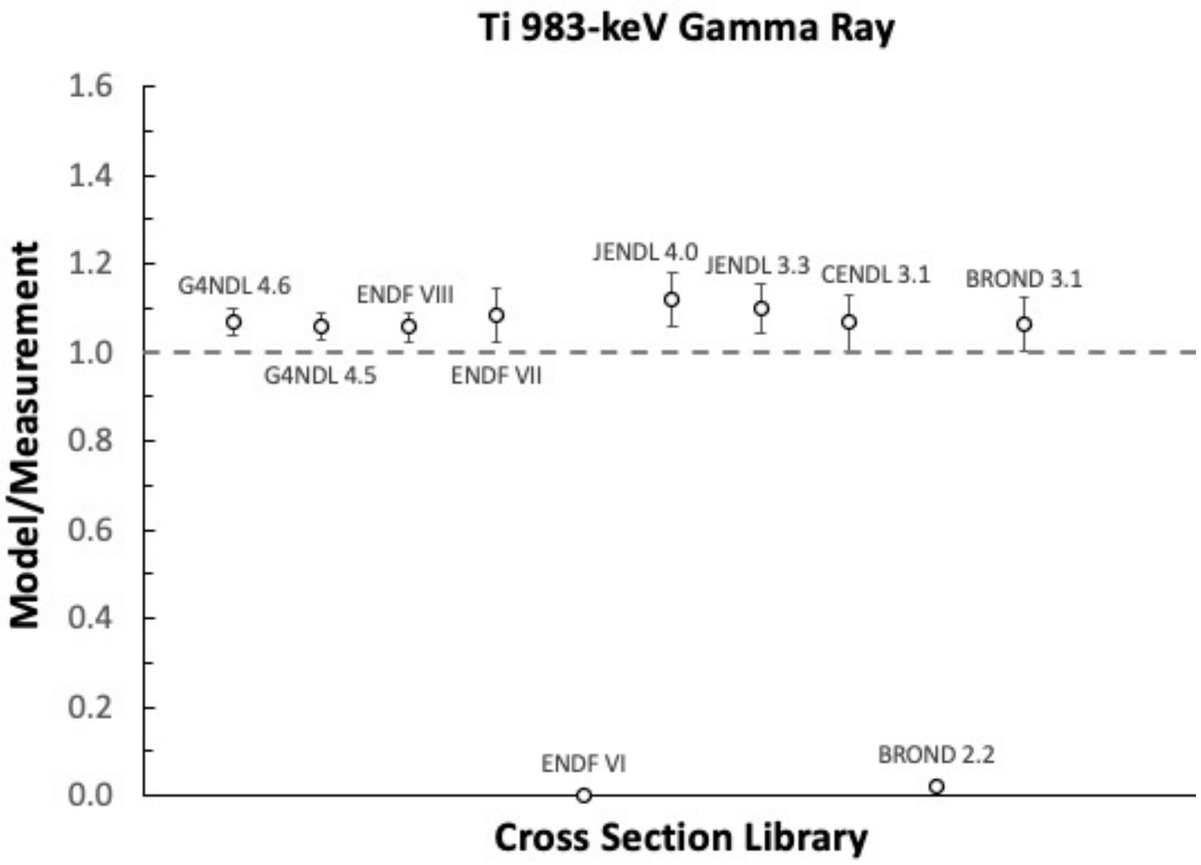
Calcium – 3736-keV gamma ray



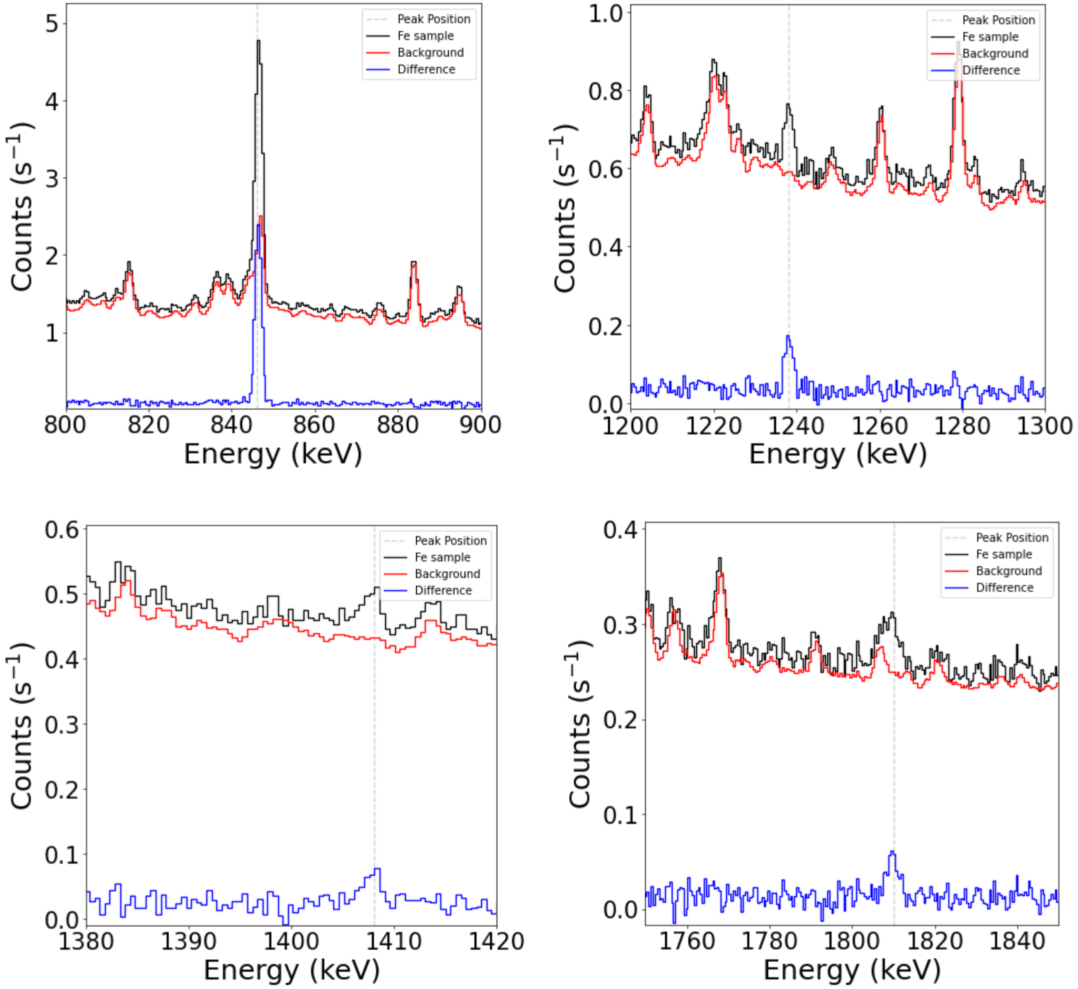


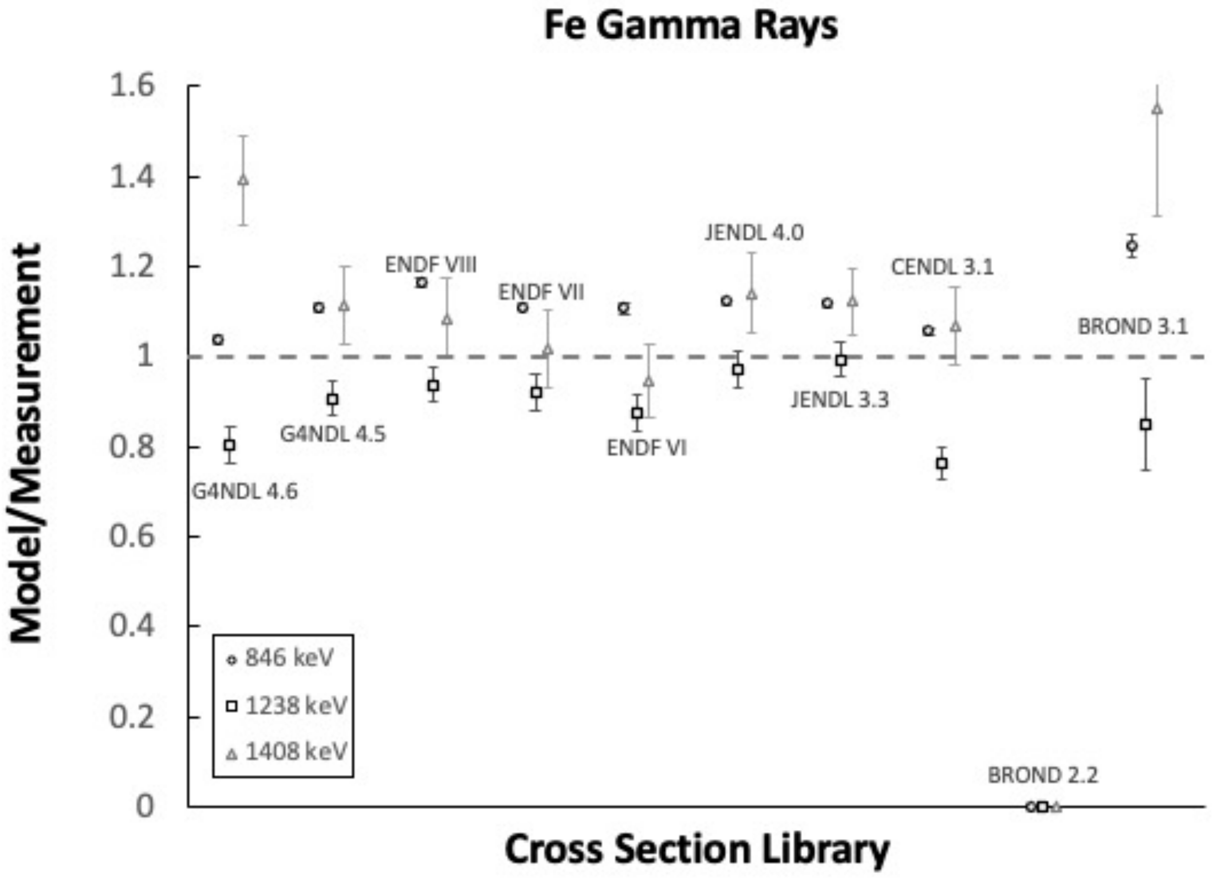
Titanium – 983-keV gamma ray



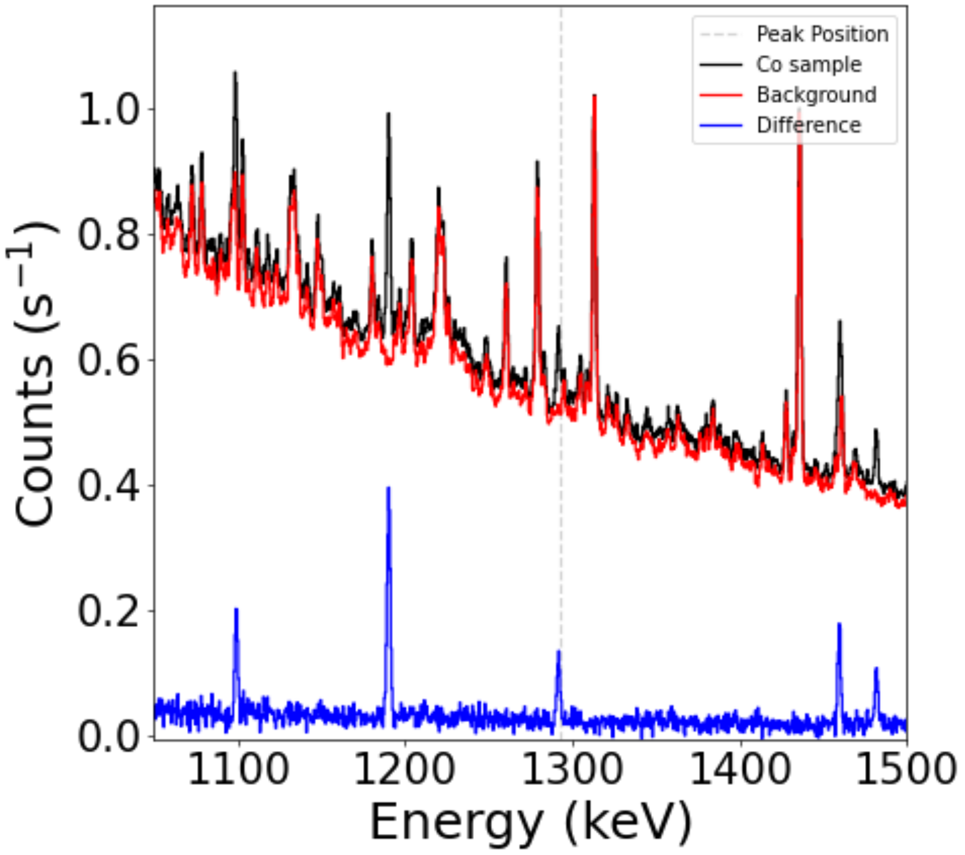


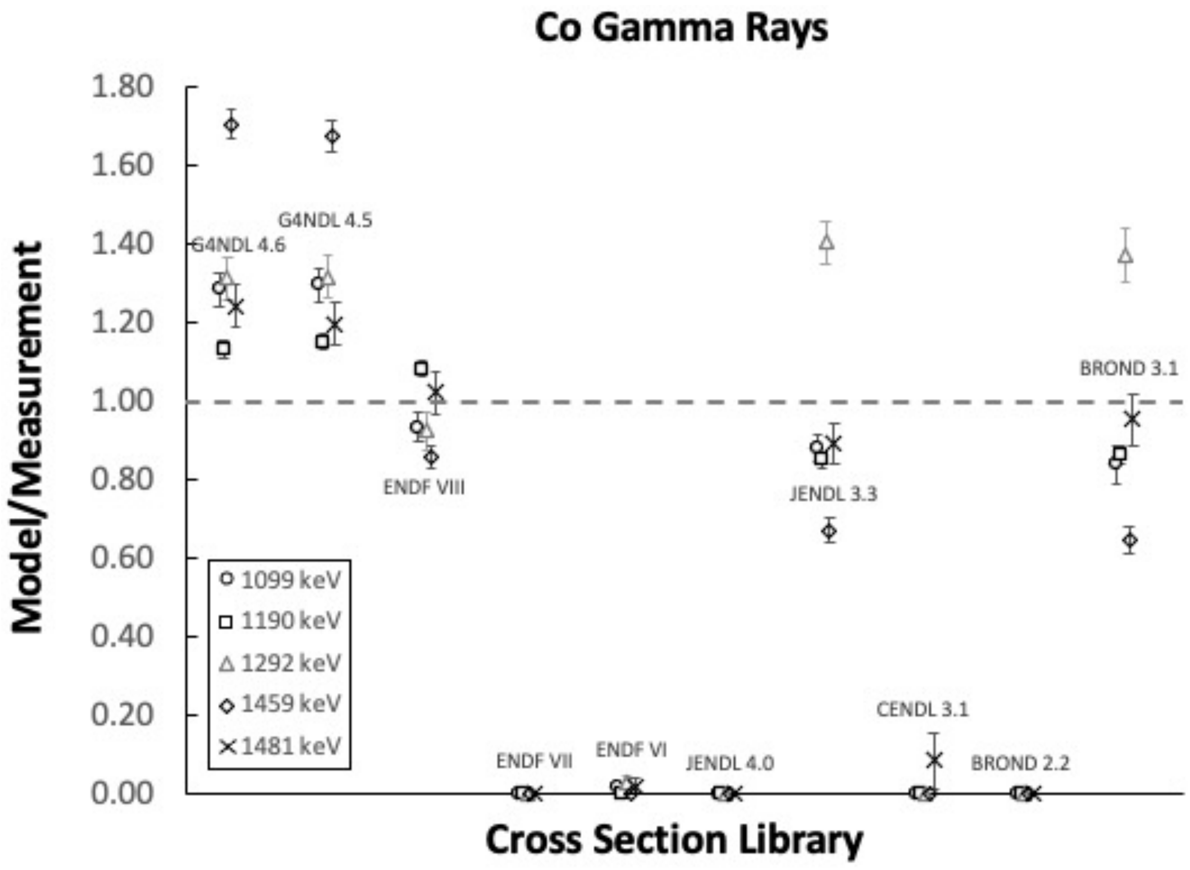
Iron – multiple gamma-ray peaks





Cobalt – multiple gamma-ray peaks





Nickel – multiple gamma-ray peaks